



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 07:26 PM EST

PDB ID : 8JR6
BMRB ID : 36575
Title : Hsp90a N-terminal domain
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Deposited on : 2023-06-16

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

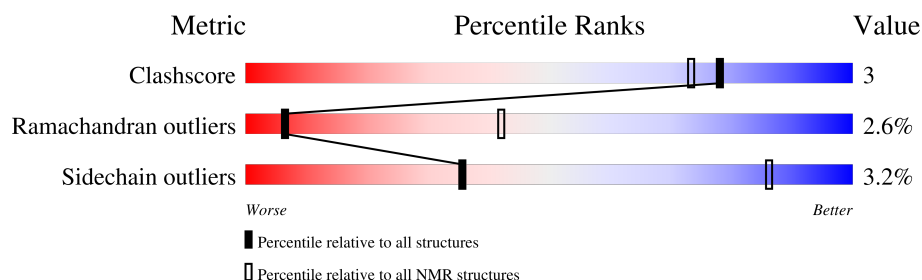
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 16%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	237	

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 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:16-A:63, A:75-A:222 (196)	1.97	6

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3717 atoms, of which 1841 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein HSP 90-alpha.

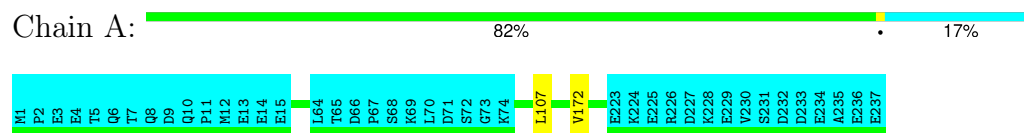
Mol	Chain	Residues	Atoms							Trace
1	A	237	Total	C	H	N	O	S		0
			3717	1176	1841	306	387	7		

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: Heat shock protein HSP 90-alpha

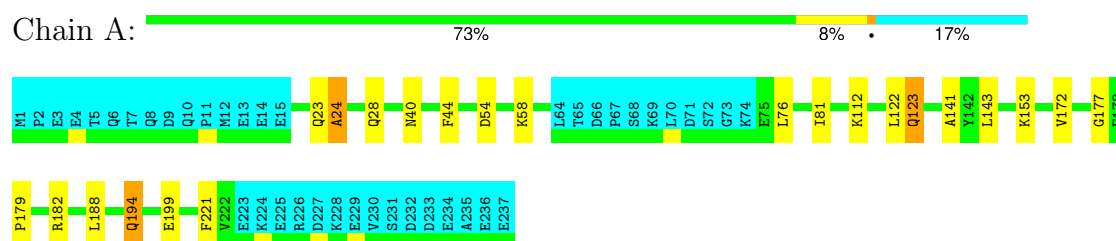


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

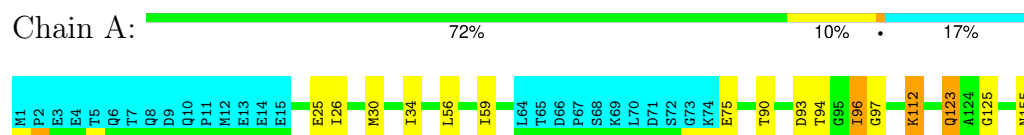
4.2.1 Score per residue for model 1

- Molecule 1: Heat shock protein HSP 90-alpha



4.2.2 Score per residue for model 2

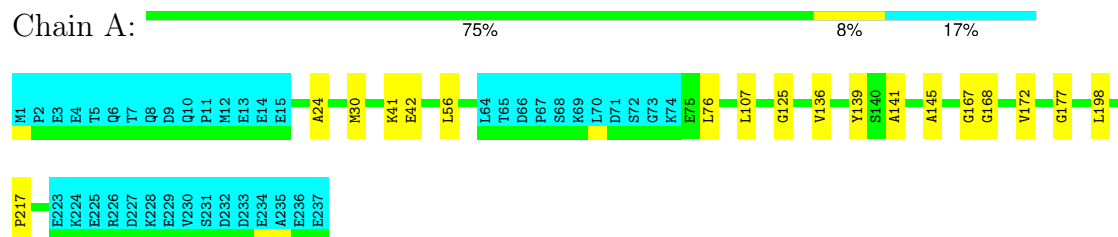
- Molecule 1: Heat shock protein HSP 90-alpha





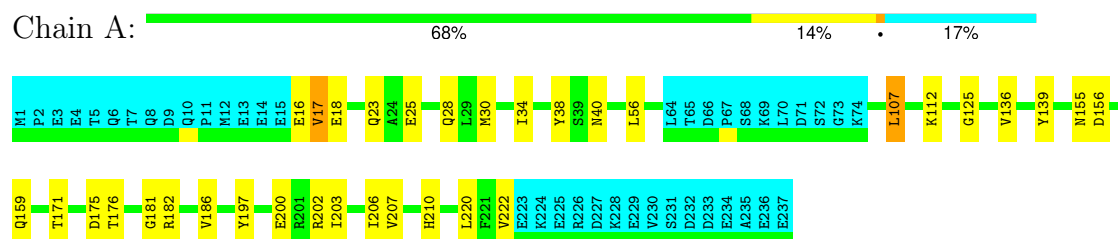
4.2.3 Score per residue for model 3

- Molecule 1: Heat shock protein HSP 90-alpha



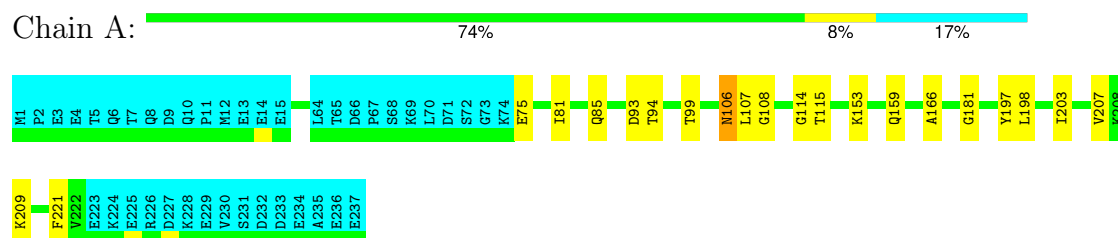
4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein HSP 90-alpha



4.2.5 Score per residue for model 5

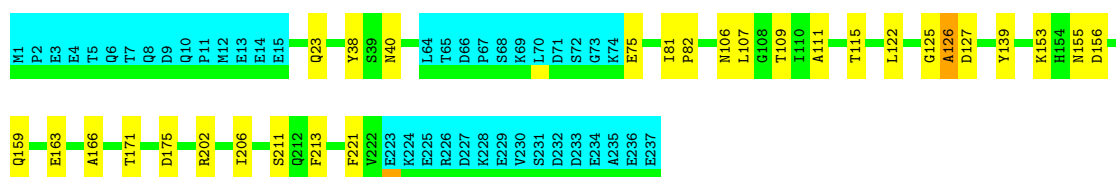
- Molecule 1: Heat shock protein HSP 90-alpha



4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Heat shock protein HSP 90-alpha





4.2.7 Score per residue for model 7

- Molecule 1: Heat shock protein HSP 90-alpha

Chain A: 74% 8% 17%



4.2.8 Score per residue for model 8

- Molecule 1: Heat shock protein HSP 90-alpha

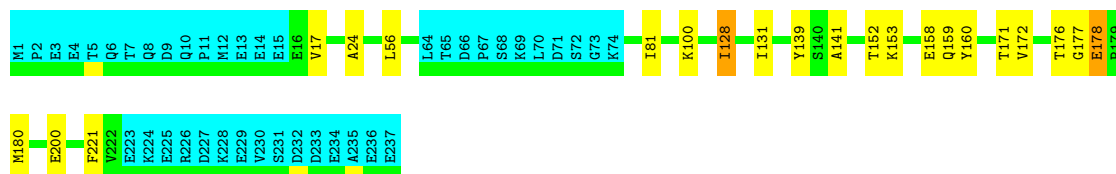
Chain A: 72% 8% 17%



4.2.9 Score per residue for model 9

- Molecule 1: Heat shock protein HSP 90-alpha

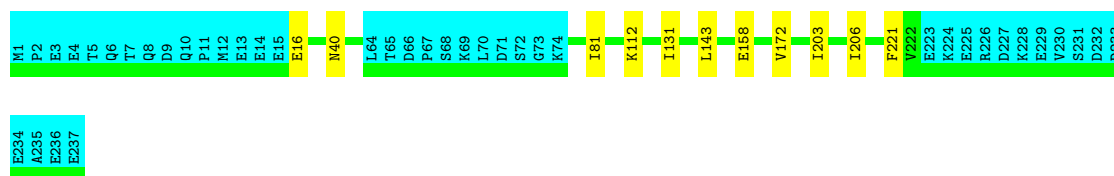
Chain A: 73% 8% 17%



4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein HSP 90-alpha

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

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

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	469
Number of shifts mapped to atoms	469
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	16%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1546	1546	1546	8±4
All	All	15460	15460	15460	84

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:ASN:O	1:A:107:LEU:HG	0.67	1.90	5	1
1:A:177:GLY:O	1:A:179:PRO:HD3	0.62	1.94	1	1
1:A:30:MET:SD	1:A:167:GLY:HA2	0.59	2.37	3	1
1:A:103:LEU:O	1:A:107:LEU:HG	0.57	2.00	8	1
1:A:141:ALA:HA	1:A:145:ALA:HB3	0.55	1.78	3	1
1:A:203:ILE:HG23	1:A:220:LEU:HD21	0.55	1.79	4	1
1:A:200:GLU:O	1:A:203:ILE:HG22	0.54	2.03	4	1
1:A:107:LEU:O	1:A:107:LEU:HD13	0.53	2.03	6	1
1:A:163:GLU:HB2	1:A:171:THR:OG1	0.52	2.04	6	2
1:A:16:GLU:O	1:A:17:VAL:HG22	0.52	2.04	4	1
1:A:153:LYS:HD2	1:A:180:MET:SD	0.52	2.45	9	1
1:A:159:GLN:HB3	1:A:175:ASP:O	0.51	2.06	6	1
1:A:150:VAL:CG2	1:A:162:TRP:HB3	0.51	2.36	7	1
1:A:38:TYR:CE2	1:A:40:ASN:HB3	0.50	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:ARG:HG3	1:A:182:ARG:O	0.49	2.07	2	1
1:A:23:GLN:OE1	1:A:111:ALA:HA	0.49	2.06	6	1
1:A:30:MET:O	1:A:34:ILE:HG12	0.49	2.07	2	2
1:A:38:TYR:CE2	1:A:40:ASN:HB2	0.49	2.43	6	1
1:A:38:TYR:CE1	1:A:143:LEU:HD12	0.49	2.42	8	1
1:A:211:SER:C	1:A:213:PHE:H	0.48	2.11	6	1
1:A:159:GLN:HG3	1:A:176:THR:C	0.48	2.29	9	1
1:A:107:LEU:HD11	1:A:162:TRP:CE2	0.47	2.45	8	1
1:A:162:TRP:CZ3	1:A:172:VAL:HG13	0.47	2.44	8	1
1:A:25:GLU:O	1:A:28:GLN:HB3	0.47	2.09	4	1
1:A:44:PHE:CZ	1:A:141:ALA:HB2	0.47	2.45	1	1
1:A:54:ASP:O	1:A:58:LYS:HG2	0.47	2.10	1	1
1:A:202:ARG:O	1:A:206:ILE:HG13	0.47	2.09	4	1
1:A:152:THR:O	1:A:159:GLN:HA	0.47	2.10	9	1
1:A:81:ILE:CG2	1:A:221:PHE:HB3	0.46	2.41	10	1
1:A:207:VAL:HB	1:A:212:GLN:NE2	0.46	2.26	2	1
1:A:43:ILE:O	1:A:47:GLU:HB2	0.46	2.11	8	1
1:A:122:LEU:HD22	1:A:127:ASP:HB2	0.46	1.86	6	1
1:A:16:GLU:H	1:A:16:GLU:CD	0.46	2.14	10	1
1:A:203:ILE:O	1:A:207:VAL:HG23	0.46	2.10	5	1
1:A:59:ILE:HB	1:A:96:ILE:H	0.45	1.71	2	1
1:A:54:ASP:O	1:A:58:LYS:HB2	0.45	2.12	7	1
1:A:81:ILE:HG22	1:A:221:PHE:HB2	0.45	1.88	1	3
1:A:155:ASN:O	1:A:156:ASP:HB3	0.45	2.11	2	2
1:A:103:LEU:HG	1:A:162:TRP:HE1	0.44	1.73	8	1
1:A:128:ILE:O	1:A:131:ILE:HG13	0.44	2.13	9	1
1:A:76:LEU:O	1:A:217:PRO:HD2	0.44	2.11	3	1
1:A:18:GLU:O	1:A:171:THR:HA	0.44	2.12	4	1
1:A:125:GLY:O	1:A:126:ALA:HB2	0.44	2.13	6	1
1:A:123:GLN:HE21	1:A:123:GLN:HA	0.43	1.73	2	2
1:A:107:LEU:HD21	1:A:162:TRP:CD1	0.43	2.48	8	1
1:A:24:ALA:O	1:A:28:GLN:HG3	0.43	2.13	1	1
1:A:26:ILE:HD11	1:A:112:LYS:HB2	0.43	1.91	2	1
1:A:207:VAL:HB	1:A:212:GLN:CD	0.43	2.34	2	1
1:A:100:LYS:HD2	1:A:160:TYR:CZ	0.43	2.48	9	1
1:A:143:LEU:O	1:A:143:LEU:HD23	0.43	2.13	1	1
1:A:75:GLU:HB2	1:A:94:THR:HG21	0.43	1.89	8	1
1:A:142:TYR:HA	1:A:145:ALA:O	0.43	2.14	8	1
1:A:181:GLY:C	1:A:182:ARG:HD3	0.43	2.34	8	1
1:A:207:VAL:HA	1:A:210:HIS:CE1	0.42	2.48	4	1
1:A:114:GLY:HA2	1:A:118:PHE:CD1	0.42	2.49	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:GLN:HE21	1:A:194:GLN:HA	0.42	1.74	1	2
1:A:198:LEU:O	1:A:198:LEU:HG	0.42	2.13	3	1
1:A:159:GLN:HG3	1:A:175:ASP:O	0.42	2.15	4	1
1:A:153:LYS:HE2	1:A:159:GLN:OE1	0.42	2.14	5	1
1:A:153:LYS:O	1:A:182:ARG:HA	0.42	2.15	1	1
1:A:90:THR:HG23	1:A:187:ILE:HG22	0.42	1.91	2	1
1:A:202:ARG:O	1:A:206:ILE:HG12	0.42	2.14	6	1
1:A:81:ILE:HG22	1:A:221:PHE:HB3	0.42	1.91	9	1
1:A:200:GLU:OE1	1:A:222:VAL:HB	0.42	2.15	4	1
1:A:153:LYS:HD3	1:A:178:GLU:O	0.41	2.14	8	1
1:A:136:VAL:HG22	1:A:136:VAL:O	0.41	2.15	3	1
1:A:118:PHE:O	1:A:122:LEU:HG	0.41	2.15	8	1
1:A:78:ILE:HG23	1:A:218:ILE:HG22	0.41	1.92	8	1
1:A:81:ILE:CG2	1:A:221:PHE:HB2	0.41	2.46	6	1
1:A:40:ASN:CB	1:A:143:LEU:HD13	0.41	2.45	10	1
1:A:155:ASN:O	1:A:156:ASP:HB2	0.41	2.16	4	1
1:A:153:LYS:HG2	1:A:159:GLN:HB2	0.41	1.90	6	1
1:A:150:VAL:HG23	1:A:162:TRP:HB3	0.41	1.93	7	1
1:A:139:TYR:C	1:A:141:ALA:H	0.41	2.20	9	1
1:A:177:GLY:O	1:A:178:GLU:HB2	0.41	2.16	9	1
1:A:203:ILE:O	1:A:206:ILE:HG22	0.40	2.16	10	1
1:A:93:ASP:OD2	1:A:94:THR:N	0.40	2.53	2	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	196/237 (83%)	170±5 (87±2%)	21±4 (11±2%)	5±2 (3±1%)	6	42
All	All	1960/2370 (83%)	1702 (87%)	208 (11%)	50 (3%)	6	42

All 28 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	24	ALA	4
1	A	112	LYS	4
1	A	125	GLY	3
1	A	168	GLY	3
1	A	139	TYR	3
1	A	181	GLY	3
1	A	96	ILE	2
1	A	178	GLU	2
1	A	17	VAL	2
1	A	75	GLU	2
1	A	106	ASN	2
1	A	166	ALA	2
1	A	126	ALA	2
1	A	158	GLU	2
1	A	40	ASN	1
1	A	25	GLU	1
1	A	97	GLY	1
1	A	177	GLY	1
1	A	107	LEU	1
1	A	136	VAL	1
1	A	108	GLY	1
1	A	114	GLY	1
1	A	197	TYR	1
1	A	113	SER	1
1	A	155	ASN	1
1	A	156	ASP	1
1	A	36	THR	1
1	A	109	THR	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	168/207 (81%)	163±2 (97±1%)	5±2 (3±1%)	36	86
All	All	1680/2070 (81%)	1626 (97%)	54 (3%)	36	86

All 35 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	172	VAL	6
1	A	56	LEU	5
1	A	115	THR	3
1	A	23	GLN	2
1	A	123	GLN	2
1	A	194	GLN	2
1	A	176	THR	2
1	A	42	GLU	2
1	A	107	LEU	2
1	A	182	ARG	2
1	A	94	THR	2
1	A	76	LEU	1
1	A	122	LEU	1
1	A	188	LEU	1
1	A	199	GLU	1
1	A	158	GLU	1
1	A	41	LYS	1
1	A	186	VAL	1
1	A	197	TYR	1
1	A	85	GLN	1
1	A	93	ASP	1
1	A	99	THR	1
1	A	198	LEU	1
1	A	209	LYS	1
1	A	75	GLU	1
1	A	109	THR	1
1	A	22	PHE	1
1	A	146	GLU	1
1	A	187	ILE	1
1	A	38	TYR	1
1	A	47	GLU	1
1	A	128	ILE	1
1	A	171	THR	1
1	A	200	GLU	1
1	A	131	ILE	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 16% for the well-defined parts and 15% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	469
Number of shifts mapped to atoms	469
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

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

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 16%, i.e. 428 atoms were assigned a chemical shift out of a possible 2683. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/988 (0%)	0/403 (0%)	0/392 (0%)	0/193 (0%)
Sidechain	428/1492 (29%)	321/972 (33%)	107/470 (23%)	0/50 (0%)
Aromatic	0/203 (0%)	0/100 (0%)	0/98 (0%)	0/5 (0%)
Overall	428/2683 (16%)	321/1475 (22%)	107/960 (11%)	0/248 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 469 atoms were assigned a chemical shift out of a possible 3198. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1188 (0%)	0/483 (0%)	0/474 (0%)	0/231 (0%)
Sidechain	469/1807 (26%)	351/1167 (30%)	118/580 (20%)	0/60 (0%)
Aromatic	0/203 (0%)	0/100 (0%)	0/98 (0%)	0/5 (0%)
Overall	469/3198 (15%)	351/1750 (20%)	118/1152 (10%)	0/296 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

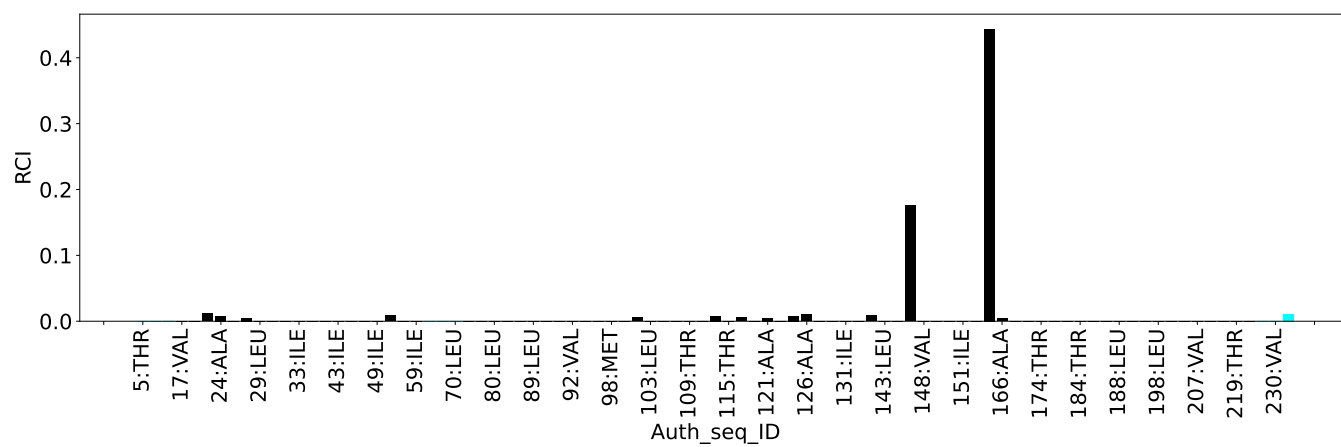
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	144	VAL	CG1	12.72	14.71 – 28.29	-6.5
1	A	107	LEU	HD11	-0.94	-0.61 – 2.12	-6.2
1	A	107	LEU	HD12	-0.94	-0.61 – 2.12	-6.2
1	A	107	LEU	HD13	-0.94	-0.61 – 2.12	-6.2
1	A	144	VAL	HG11	-0.71	-0.48 – 2.12	-5.9
1	A	144	VAL	HG12	-0.71	-0.48 – 2.12	-5.9
1	A	144	VAL	HG13	-0.71	-0.48 – 2.12	-5.9
1	A	107	LEU	HD21	-0.73	-0.65 – 2.13	-5.3
1	A	107	LEU	HD22	-0.73	-0.65 – 2.13	-5.3
1	A	107	LEU	HD23	-0.73	-0.65 – 2.13	-5.3

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	1264
Intra-residue ($ i-j =0$)	104
Sequential ($ i-j =1$)	285
Medium range ($ i-j >1$ and $ i-j <5$)	281
Long range ($ i-j \geq 5$)	444
Inter-chain	0
Hydrogen bond restraints	150
Disulfide bond restraints	0
Total dihedral-angle restraints	298
Number of unmapped restraints	0
Number of restraints per residue	6.6
Number of long range restraints per residue ¹	2.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	77.8	0.2
0.2-0.5 (Medium)	44.9	0.5
>0.5 (Large)	1.2	0.7

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)	15.2	6.68
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

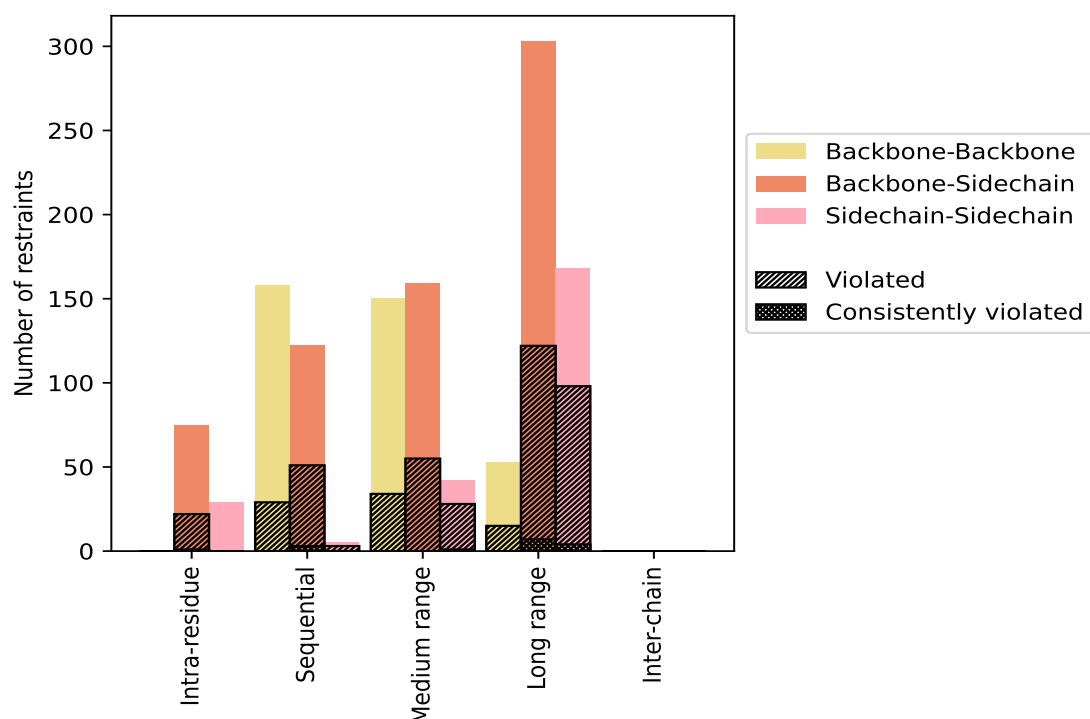
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	104	8.2	22	21.2	1.7	1	1.0	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	75	5.9	22	29.3	1.7	1	1.3	0.1
Sidechain-Sidechain	29	2.3	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	285	22.5	83	29.1	6.6	3	1.1	0.2
Backbone-Backbone	158	12.5	29	18.4	2.3	0	0.0	0.0
Backbone-Sidechain	122	9.7	51	41.8	4.0	3	2.5	0.2
Sidechain-Sidechain	5	0.4	3	60.0	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	281	22.2	106	37.7	8.4	1	0.4	0.1
Backbone-Backbone	150	11.9	34	22.7	2.7	0	0.0	0.0
Backbone-Sidechain	89	7.0	44	49.4	3.5	0	0.0	0.0
Sidechain-Sidechain	42	3.3	28	66.7	2.2	1	2.4	0.1
Long range ($i-j \geq 5$)	444	35.1	221	49.8	17.5	10	2.3	0.8
Backbone-Backbone	53	4.2	15	28.3	1.2	0	0.0	0.0
Backbone-Sidechain	223	17.6	108	48.4	8.5	6	2.7	0.5
Sidechain-Sidechain	168	13.3	98	58.3	7.8	4	2.4	0.3
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	150	11.9	25	16.7	2.0	1	0.7	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1264	100.0	457	36.2	36.2	16	1.3	1.3
Backbone-Backbone	361	28.6	78	21.6	6.2	0	0.0	0.0
Backbone-Sidechain	659	52.1	250	37.9	19.8	11	1.7	0.9
Sidechain-Sidechain	244	19.3	129	52.9	10.2	5	2.0	0.4

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

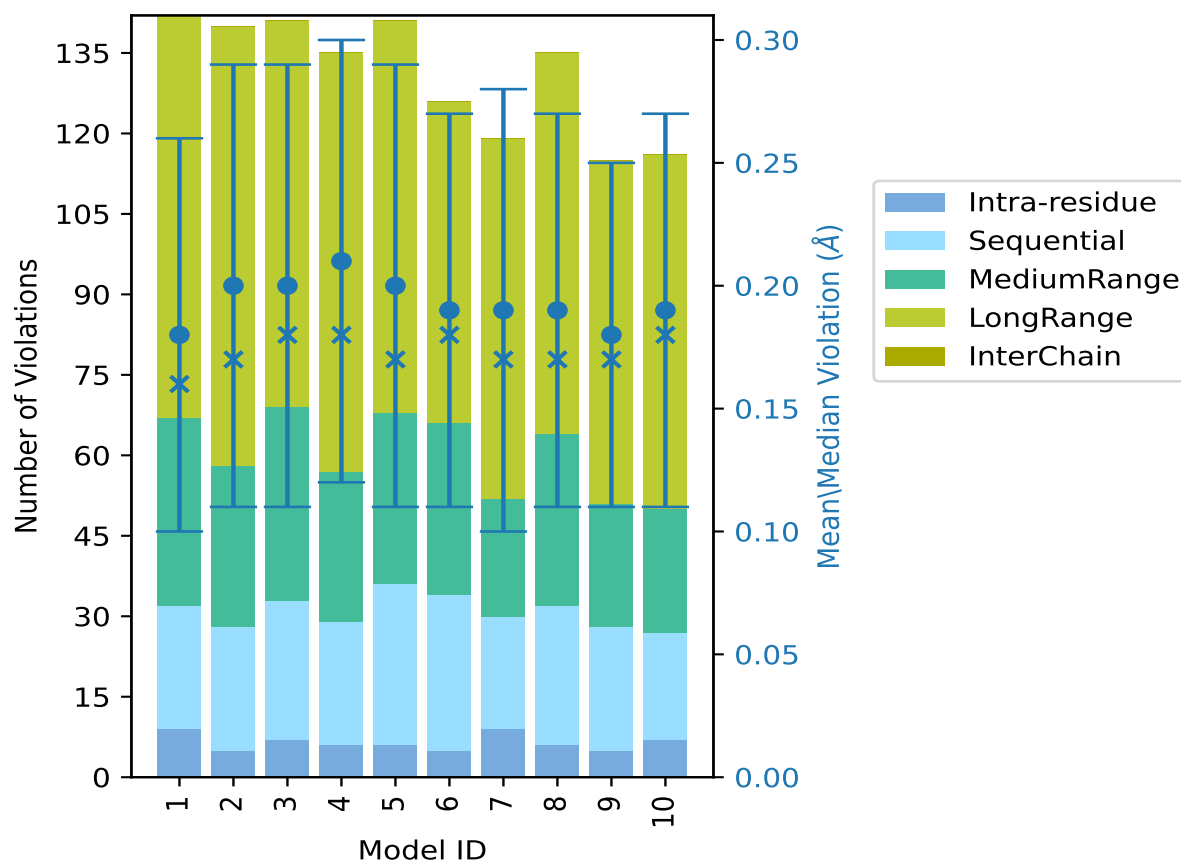
9.2 Distance violation statistics for each model [i](#)

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	9	23	35	75	0	142	0.18	0.52	0.08	0.16
2	5	23	30	82	0	140	0.2	0.51	0.09	0.17
3	7	26	36	72	0	141	0.2	0.63	0.09	0.18
4	6	23	28	78	0	135	0.21	0.55	0.09	0.18
5	6	30	32	73	0	141	0.2	0.55	0.09	0.17
6	5	29	32	60	0	126	0.19	0.66	0.08	0.18
7	9	21	22	67	0	119	0.19	0.51	0.09	0.17
8	6	26	32	71	0	135	0.19	0.52	0.08	0.17
9	5	23	23	64	0	115	0.18	0.42	0.07	0.17
10	7	20	23	66	0	116	0.19	0.7	0.08	0.18

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 682(IR:82, SQ:202, MR:175, LR:223, 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	%
9	33	39	74	0	155	1	10.0
3	16	28	54	0	101	2	20.0
4	11	14	31	0	60	3	30.0

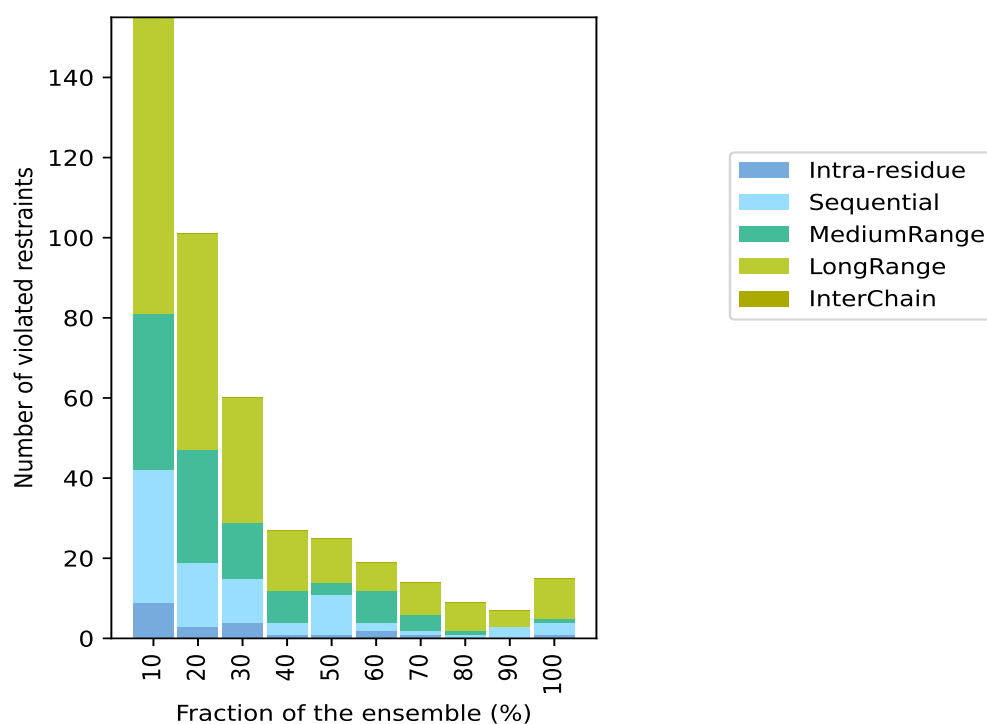
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	3	8	15	0	27	4	40.0
1	10	3	11	0	25	5	50.0
2	2	8	7	0	19	6	60.0
1	1	4	8	0	14	7	70.0
0	1	1	7	0	9	8	80.0
0	3	0	4	0	7	9	90.0
1	3	1	10	0	15	10	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

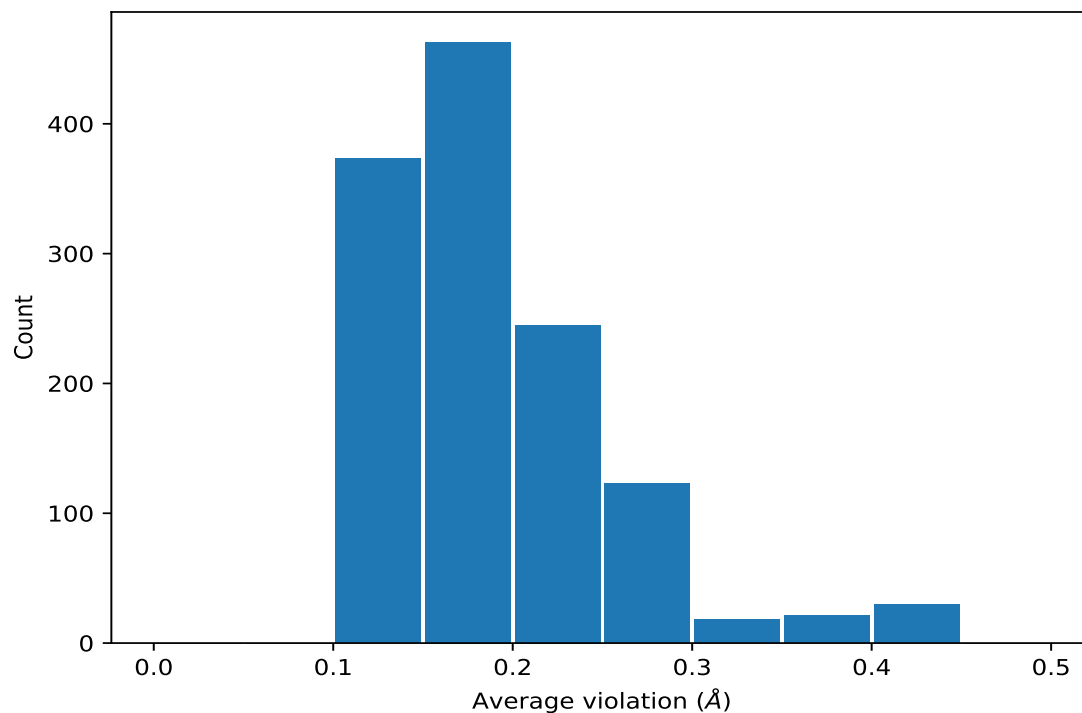


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	10	0.4	0.06	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	10	0.4	0.06	0.42
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	10	0.37	0.08	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	10	0.37	0.08	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	10	0.37	0.08	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	10	0.37	0.08	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	10	0.37	0.08	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	10	0.37	0.08	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	10	0.37	0.08	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	10	0.37	0.08	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	10	0.37	0.08	0.34
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	10	0.28	0.05	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	10	0.28	0.05	0.29
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	10	0.27	0.07	0.26
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	10	0.27	0.07	0.26
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	10	0.27	0.07	0.26
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	10	0.27	0.05	0.26
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	10	0.27	0.05	0.26
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	10	0.27	0.05	0.26
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	10	0.25	0.04	0.24
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	10	0.25	0.04	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	10	0.23	0.06	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	10	0.23	0.06	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	10	0.23	0.06	0.24
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	10	0.23	0.11	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	10	0.23	0.11	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	10	0.23	0.11	0.18
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	10	0.22	0.06	0.23
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	10	0.22	0.06	0.23
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	10	0.22	0.06	0.23
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	10	0.22	0.06	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	10	0.22	0.06	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	10	0.22	0.06	0.22
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	10	0.21	0.04	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	10	0.21	0.04	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	10	0.21	0.04	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	10	0.2	0.04	0.2
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	10	0.2	0.04	0.2
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	10	0.2	0.04	0.2
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	10	0.2	0.05	0.19
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	10	0.2	0.05	0.19
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	10	0.2	0.05	0.19
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	10	0.17	0.04	0.16
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	10	0.17	0.04	0.16
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	10	0.17	0.04	0.16
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	10	0.16	0.03	0.16
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	10	0.16	0.03	0.16
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	10	0.14	0.03	0.14
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	9	0.26	0.07	0.25
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	9	0.26	0.07	0.25
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	9	0.26	0.07	0.25
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	9	0.25	0.08	0.26
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	9	0.25	0.08	0.26
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	9	0.25	0.08	0.26
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	9	0.25	0.07	0.27
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	9	0.25	0.07	0.27
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	9	0.21	0.06	0.22
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	9	0.21	0.06	0.22
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	9	0.21	0.06	0.22
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	9	0.18	0.04	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	9	0.18	0.04	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	9	0.18	0.04	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	9	0.18	0.03	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	9	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	9	0.18	0.03	0.18
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	9	0.16	0.05	0.14
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	9	0.16	0.05	0.14
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	9	0.16	0.05	0.14
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	8	0.24	0.11	0.22
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	8	0.24	0.11	0.22
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	8	0.23	0.08	0.23
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	8	0.23	0.08	0.23
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	8	0.23	0.08	0.23
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	8	0.22	0.09	0.22
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	8	0.22	0.09	0.22
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	8	0.2	0.06	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	8	0.2	0.06	0.18
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	8	0.2	0.06	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	8	0.2	0.06	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	8	0.2	0.06	0.19
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	8	0.18	0.03	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	8	0.18	0.03	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	8	0.18	0.03	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	8	0.18	0.03	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	8	0.18	0.03	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	8	0.18	0.03	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	8	0.18	0.03	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	8	0.18	0.03	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	8	0.18	0.03	0.17
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	8	0.18	0.04	0.18
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	8	0.18	0.04	0.18
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	8	0.14	0.02	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	8	0.14	0.02	0.12
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	8	0.14	0.02	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	8	0.14	0.02	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	8	0.14	0.02	0.13
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	7	0.26	0.19	0.17
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	7	0.26	0.19	0.17
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	7	0.25	0.13	0.21
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	7	0.25	0.13	0.21
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	7	0.25	0.13	0.21
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	7	0.25	0.13	0.21
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	7	0.25	0.13	0.21
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	7	0.25	0.13	0.21
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	7	0.25	0.13	0.21
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	7	0.25	0.13	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	7	0.25	0.13	0.21
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	7	0.23	0.04	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	7	0.23	0.04	0.22
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	7	0.21	0.04	0.2
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	7	0.21	0.04	0.2
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	7	0.21	0.06	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	7	0.21	0.06	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	7	0.21	0.06	0.23
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	7	0.2	0.06	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	7	0.2	0.06	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	7	0.2	0.06	0.21
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	7	0.19	0.04	0.19
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	7	0.19	0.04	0.19
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	7	0.19	0.04	0.19
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	7	0.19	0.03	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	7	0.19	0.03	0.21
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	7	0.19	0.04	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	7	0.19	0.04	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	7	0.19	0.04	0.18
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	7	0.17	0.07	0.14
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	7	0.17	0.07	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	7	0.17	0.07	0.14
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	7	0.17	0.04	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	7	0.17	0.04	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	7	0.17	0.04	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	7	0.17	0.03	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	7	0.17	0.03	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	7	0.17	0.03	0.17
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	7	0.16	0.04	0.14
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	7	0.16	0.04	0.14
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	7	0.15	0.04	0.14
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	7	0.15	0.04	0.14
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	7	0.15	0.04	0.14
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	6	0.41	0.05	0.4
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG21	6	0.24	0.05	0.24
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG22	6	0.24	0.05	0.24
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG23	6	0.24	0.05	0.24
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB1	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB2	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB3	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB1	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB2	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB3	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB1	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB2	6	0.22	0.08	0.23
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB3	6	0.22	0.08	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	6	0.22	0.04	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	6	0.22	0.04	0.23
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB1	6	0.21	0.1	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB2	6	0.21	0.1	0.17
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB3	6	0.21	0.1	0.17
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD11	6	0.2	0.04	0.19
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD12	6	0.2	0.04	0.19
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD13	6	0.2	0.04	0.19
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	6	0.19	0.05	0.2
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	6	0.19	0.05	0.2
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	6	0.19	0.05	0.18
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	6	0.19	0.05	0.18
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	6	0.18	0.06	0.16
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	6	0.18	0.06	0.16
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD21	6	0.18	0.06	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD22	6	0.18	0.06	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD23	6	0.18	0.06	0.15
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	6	0.18	0.08	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	6	0.18	0.08	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	6	0.18	0.08	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	6	0.18	0.08	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	6	0.18	0.08	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	6	0.18	0.08	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	6	0.18	0.08	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	6	0.18	0.08	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	6	0.18	0.08	0.13
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG21	6	0.17	0.05	0.18
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG22	6	0.17	0.05	0.18
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG23	6	0.17	0.05	0.18
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG21	6	0.17	0.03	0.17
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG22	6	0.17	0.03	0.17
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG23	6	0.17	0.03	0.17
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG11	6	0.16	0.04	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG12	6	0.16	0.04	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG13	6	0.16	0.04	0.18
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	6	0.15	0.03	0.15
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	6	0.15	0.03	0.15
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	6	0.14	0.05	0.12
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	6	0.14	0.05	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	6	0.14	0.03	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	6	0.14	0.03	0.12
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD11	6	0.14	0.02	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD12	6	0.14	0.02	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD13	6	0.14	0.02	0.13
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD11	6	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD12	6	0.12	0.02	0.11
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD13	6	0.12	0.02	0.11
(1,87)	1:137:A:GLY:H	1:138:A:PHE:H	5	0.4	0.19	0.31
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG12	5	0.33	0.05	0.35
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG13	5	0.33	0.05	0.35
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD11	5	0.29	0.16	0.29
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD12	5	0.29	0.16	0.29
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD13	5	0.29	0.16	0.29
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB1	5	0.25	0.07	0.26
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB2	5	0.25	0.07	0.26
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB3	5	0.25	0.07	0.26
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB1	5	0.25	0.06	0.21
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB2	5	0.25	0.06	0.21
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB3	5	0.25	0.06	0.21
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG21	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG22	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG23	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG21	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG22	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG23	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG21	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG22	5	0.25	0.08	0.25
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG23	5	0.25	0.08	0.25
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD21	5	0.24	0.03	0.23
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD22	5	0.24	0.03	0.23
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD23	5	0.24	0.03	0.23
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	5	0.22	0.05	0.22
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	5	0.22	0.05	0.22
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB1	5	0.21	0.06	0.23
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB2	5	0.21	0.06	0.23
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB3	5	0.21	0.06	0.23
(1,693)	1:31:A:SER:H	1:30:A:MET:HE1	5	0.21	0.07	0.17
(1,693)	1:31:A:SER:H	1:30:A:MET:HE2	5	0.21	0.07	0.17
(1,693)	1:31:A:SER:H	1:30:A:MET:HE3	5	0.21	0.07	0.17
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	5	0.2	0.08	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	5	0.2	0.08	0.17
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	5	0.2	0.08	0.17
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	5	0.2	0.08	0.17
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	5	0.2	0.08	0.17
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	5	0.2	0.08	0.17
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	5	0.2	0.08	0.17
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	5	0.2	0.08	0.17
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	5	0.2	0.08	0.17
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	5	0.19	0.04	0.18
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	5	0.19	0.04	0.18
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	5	0.19	0.04	0.18
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD21	5	0.19	0.04	0.21
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD22	5	0.19	0.04	0.21
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD23	5	0.19	0.04	0.21
(1,69)	1:105:A:ASN:H	1:106:A:ASN:H	5	0.19	0.05	0.19
(1,277)	1:131:A:ILE:H	1:134:A:PHE:H	5	0.18	0.07	0.15
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	5	0.17	0.04	0.17
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	5	0.17	0.04	0.17
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG21	5	0.17	0.04	0.18
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG22	5	0.17	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG23	5	0.17	0.04	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG11	5	0.17	0.03	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG12	5	0.17	0.03	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG13	5	0.17	0.03	0.18
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG21	5	0.16	0.04	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG22	5	0.16	0.04	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG23	5	0.16	0.04	0.15
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG11	5	0.15	0.02	0.15
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG12	5	0.15	0.02	0.15
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG13	5	0.15	0.02	0.15
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD11	5	0.15	0.05	0.13
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD12	5	0.15	0.05	0.13
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD13	5	0.15	0.05	0.13
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	5	0.14	0.04	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	5	0.14	0.04	0.12
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD11	5	0.13	0.02	0.12
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD12	5	0.13	0.02	0.12
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD13	5	0.13	0.02	0.12
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB1	5	0.12	0.03	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB2	5	0.12	0.03	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB3	5	0.12	0.03	0.1
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG21	4	0.4	0.07	0.4
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG22	4	0.4	0.07	0.4
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG23	4	0.4	0.07	0.4
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	4	0.32	0.08	0.34
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	4	0.32	0.08	0.34
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG21	4	0.27	0.07	0.3
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG22	4	0.27	0.07	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG23	4	0.27	0.07	0.3
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD11	4	0.26	0.1	0.26
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD12	4	0.26	0.1	0.26
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD13	4	0.26	0.1	0.26
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD11	4	0.22	0.06	0.2
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD12	4	0.22	0.06	0.2
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD13	4	0.22	0.06	0.2
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD11	4	0.22	0.07	0.19
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD12	4	0.22	0.07	0.19
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD13	4	0.22	0.07	0.19
(1,337)	1:103:A:LEU:H	1:107:A:LEU:H	4	0.22	0.09	0.22
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD11	4	0.21	0.07	0.22
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD12	4	0.21	0.07	0.22
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD13	4	0.21	0.07	0.22
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD21	4	0.21	0.02	0.22
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD22	4	0.21	0.02	0.22
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD23	4	0.21	0.02	0.22
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	4	0.2	0.05	0.2
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB1	4	0.2	0.02	0.2
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB2	4	0.2	0.02	0.2
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB3	4	0.2	0.02	0.2
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	4	0.19	0.03	0.2
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	4	0.19	0.03	0.2
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD11	4	0.19	0.04	0.18
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD12	4	0.19	0.04	0.18
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD13	4	0.19	0.04	0.18
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD11	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD12	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD13	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD11	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD12	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD13	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD11	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD12	4	0.19	0.05	0.18
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD13	4	0.19	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG21	4	0.19	0.05	0.2
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG22	4	0.19	0.05	0.2
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG23	4	0.19	0.05	0.2
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE1	4	0.18	0.04	0.2
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE2	4	0.18	0.04	0.2
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE3	4	0.18	0.04	0.2
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE1	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE2	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE3	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE1	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE2	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE3	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE1	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE2	4	0.18	0.04	0.18
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE3	4	0.18	0.04	0.18
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG21	4	0.18	0.07	0.15
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG22	4	0.18	0.07	0.15
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG23	4	0.18	0.07	0.15
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG21	4	0.18	0.05	0.16
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG22	4	0.18	0.05	0.16
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG23	4	0.18	0.05	0.16
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD11	4	0.17	0.06	0.14
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD12	4	0.17	0.06	0.14
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD13	4	0.17	0.06	0.14
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG21	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG22	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG23	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG21	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG22	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG23	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG21	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG22	4	0.16	0.06	0.16
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG23	4	0.16	0.06	0.16
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	4	0.16	0.03	0.15
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	4	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB1	4	0.16	0.05	0.16
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB2	4	0.16	0.05	0.16
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB3	4	0.16	0.05	0.16
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	4	0.15	0.06	0.13
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	4	0.15	0.06	0.13
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG21	4	0.15	0.02	0.15
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG22	4	0.15	0.02	0.15
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG23	4	0.15	0.02	0.15
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	4	0.14	0.02	0.15
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG21	4	0.14	0.04	0.12
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG22	4	0.14	0.04	0.12
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG23	4	0.14	0.04	0.12
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB1	4	0.13	0.03	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB2	4	0.13	0.03	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB3	4	0.13	0.03	0.11
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD11	3	0.31	0.03	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD12	3	0.31	0.03	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD13	3	0.31	0.03	0.29
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB1	3	0.26	0.1	0.23
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB2	3	0.26	0.1	0.23
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB3	3	0.26	0.1	0.23
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG21	3	0.26	0.08	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG22	3	0.26	0.08	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG23	3	0.26	0.08	0.2
(1,287)	1:194:A:GLN:H	1:197:A:TYR:H	3	0.25	0.11	0.21
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	3	0.25	0.11	0.2
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	3	0.25	0.11	0.2
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG11	3	0.25	0.11	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG12	3	0.25	0.11	0.19
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG13	3	0.25	0.11	0.19
(1,109)	1:167:A:GLY:H	1:168:A:GLY:H	3	0.24	0.09	0.19
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG11	3	0.24	0.03	0.24
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG12	3	0.24	0.03	0.24
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG13	3	0.24	0.03	0.24
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD11	3	0.24	0.07	0.21
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD12	3	0.24	0.07	0.21
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD13	3	0.24	0.07	0.21
(1,116)	1:176:A:THR:H	1:177:A:GLY:H	3	0.24	0.12	0.16
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG21	3	0.24	0.07	0.28
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG22	3	0.24	0.07	0.28
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG23	3	0.24	0.07	0.28
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD11	3	0.22	0.01	0.23
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD12	3	0.22	0.01	0.23
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD13	3	0.22	0.01	0.23
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG21	3	0.22	0.08	0.24
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG22	3	0.22	0.08	0.24
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG23	3	0.22	0.08	0.24
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG11	3	0.21	0.03	0.21
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG12	3	0.21	0.03	0.21
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG13	3	0.21	0.03	0.21
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD11	3	0.2	0.05	0.17
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD12	3	0.2	0.05	0.17
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD13	3	0.2	0.05	0.17
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD21	3	0.2	0.13	0.11
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD22	3	0.2	0.13	0.11
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD23	3	0.2	0.13	0.11
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD21	3	0.2	0.02	0.21
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD22	3	0.2	0.02	0.21
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD23	3	0.2	0.02	0.21
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	3	0.2	0.04	0.2
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	3	0.2	0.04	0.2
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG11	3	0.2	0.04	0.21
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG12	3	0.2	0.04	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG13	3	0.2	0.04	0.21
(1,167)	1:41:A:LYS:H	1:43:A:ILE:H	3	0.19	0.02	0.2
(1,288)	1:196:A:GLU:H	1:199:A:GLU:H	3	0.19	0.03	0.18
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG21	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG22	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG23	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG21	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG22	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG23	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG21	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG22	3	0.19	0.05	0.21
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG23	3	0.19	0.05	0.21
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB1	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB2	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB3	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB1	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB2	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB3	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB1	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB2	3	0.19	0.04	0.16
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB3	3	0.19	0.04	0.16
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG21	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG22	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG23	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG21	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG22	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG23	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG21	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG22	3	0.19	0.08	0.14
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG23	3	0.19	0.08	0.14
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD21	3	0.19	0.06	0.19
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD22	3	0.19	0.06	0.19
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD23	3	0.19	0.06	0.19
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE1	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE2	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE3	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE1	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE2	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE3	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE1	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE2	3	0.19	0.04	0.21
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE3	3	0.19	0.04	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD11	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD12	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD13	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD11	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD12	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD13	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD11	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD12	3	0.18	0.04	0.21
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD13	3	0.18	0.04	0.21
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG11	3	0.18	0.02	0.18
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG12	3	0.18	0.02	0.18
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG13	3	0.18	0.02	0.18
(1,263)	1:69:A:LYS:H	1:72:A:SER:H	3	0.18	0.02	0.17
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG21	3	0.18	0.02	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG22	3	0.18	0.02	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG23	3	0.18	0.02	0.16
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG11	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG12	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG13	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG11	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG12	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG13	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG11	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG12	3	0.17	0.03	0.16
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG13	3	0.17	0.03	0.16
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	3	0.17	0.07	0.13
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE1	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE2	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE3	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE1	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE2	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE3	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE1	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE2	3	0.16	0.02	0.16
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE3	3	0.16	0.02	0.16
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG21	3	0.16	0.03	0.18
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG22	3	0.16	0.03	0.18
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG23	3	0.16	0.03	0.18
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	3	0.16	0.04	0.16
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	3	0.16	0.04	0.16
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	3	0.16	0.04	0.16
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	3	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	3	0.16	0.04	0.16
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	3	0.16	0.04	0.16
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	3	0.16	0.04	0.16
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	3	0.16	0.04	0.16
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	3	0.16	0.04	0.16
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB1	3	0.15	0.03	0.15
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB2	3	0.15	0.03	0.15
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB3	3	0.15	0.03	0.15
(2,98)	1:44:A:PHE:H	1:41:A:LYS:O	3	0.15	0.03	0.14
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG21	3	0.15	0.02	0.15
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG22	3	0.15	0.02	0.15
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG23	3	0.15	0.02	0.15
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG11	3	0.15	0.02	0.16
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG12	3	0.15	0.02	0.16
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG13	3	0.15	0.02	0.16
(1,110)	1:168:A:GLY:H	1:169:A:SER:H	3	0.15	0.02	0.15
(1,314)	1:58:A:LYS:H	1:96:A:ILE:H	3	0.15	0.03	0.16
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	3	0.15	0.04	0.13
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	3	0.15	0.04	0.13
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD21	3	0.15	0.03	0.15
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD22	3	0.15	0.03	0.15
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD23	3	0.15	0.03	0.15
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD21	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD22	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD23	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD21	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD22	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD23	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD21	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD22	3	0.14	0.03	0.14
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD23	3	0.14	0.03	0.14
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD11	3	0.14	0.03	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD12	3	0.14	0.03	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD13	3	0.14	0.03	0.12
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG21	3	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG22	3	0.14	0.02	0.13
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG23	3	0.14	0.02	0.13
(1,16)	1:38:A:TYR:H	1:39:A:SER:H	3	0.13	0.04	0.11
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD11	3	0.13	0.01	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD12	3	0.13	0.01	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD13	3	0.13	0.01	0.14
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD21	3	0.13	0.01	0.13
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD22	3	0.13	0.01	0.13
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD23	3	0.13	0.01	0.13
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG21	3	0.13	0.01	0.14
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG22	3	0.13	0.01	0.14
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG23	3	0.13	0.01	0.14
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	3	0.13	0.02	0.12
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	3	0.13	0.02	0.12
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD11	3	0.12	0.01	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD12	3	0.12	0.01	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD13	3	0.12	0.01	0.13
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG21	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG22	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG23	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG21	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG22	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG23	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG21	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG22	3	0.12	0.0	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG23	3	0.12	0.0	0.12
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE1	3	0.12	0.01	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE2	3	0.12	0.01	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE3	3	0.12	0.01	0.11
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB1	3	0.12	0.02	0.11
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB2	3	0.12	0.02	0.11
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB3	3	0.12	0.02	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD11	3	0.12	0.01	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD12	3	0.12	0.01	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD13	3	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG21	3	0.12	0.01	0.12
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG22	3	0.12	0.01	0.12
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG23	3	0.12	0.01	0.12
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG11	3	0.11	0.0	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG12	3	0.11	0.0	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG13	3	0.11	0.0	0.11
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD21	3	0.11	0.01	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD22	3	0.11	0.01	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD23	3	0.11	0.01	0.1
(1,151)	1:215:A:GLY:H	1:216:A:TYR:H	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD11	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD12	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD13	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD11	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD12	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD13	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD11	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD12	3	0.11	0.01	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD13	3	0.11	0.01	0.1
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG11	2	0.44	0.09	0.44
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG12	2	0.44	0.09	0.44
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG13	2	0.44	0.09	0.44
(1,108)	1:166:A:ALA:H	1:167:A:GLY:H	2	0.42	0.01	0.42
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD11	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD12	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD13	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD11	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD12	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD13	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD11	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD12	2	0.41	0.13	0.41
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD13	2	0.41	0.13	0.41
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG11	2	0.4	0.0	0.4
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG12	2	0.4	0.0	0.4
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG13	2	0.4	0.0	0.4
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	2	0.38	0.26	0.38
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	2	0.38	0.26	0.38
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	2	0.38	0.26	0.38
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	2	0.38	0.26	0.38
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	2	0.38	0.26	0.38
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	2	0.38	0.26	0.38
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	2	0.38	0.26	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	2	0.38	0.26	0.38
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	2	0.38	0.26	0.38
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD11	2	0.37	0.14	0.37
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD12	2	0.37	0.14	0.37
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD13	2	0.37	0.14	0.37
(1,312)	1:55:A:ALA:H	1:96:A:ILE:H	2	0.32	0.06	0.32
(1,101)	1:158:A:GLU:H	1:159:A:GLN:H	2	0.32	0.06	0.32
(1,281)	1:138:A:PHE:H	1:141:A:ALA:H	2	0.32	0.01	0.32
(1,118)	1:181:A:GLY:H	1:182:A:ARG:H	2	0.31	0.03	0.31
(1,219)	1:164:A:SER:H	1:166:A:ALA:H	2	0.3	0.18	0.3
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG21	2	0.3	0.14	0.3
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG22	2	0.3	0.14	0.3
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG23	2	0.3	0.14	0.3
(1,131)	1:195:A:THR:H	1:196:A:GLU:H	2	0.29	0.08	0.29
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	2	0.28	0.18	0.28
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	2	0.28	0.18	0.28
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG11	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG12	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG13	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG11	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG12	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG13	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG11	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG12	2	0.25	0.12	0.25
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG13	2	0.25	0.12	0.25
(2,70)	1:183:A:GLY:H	1:153:A:LYS:O	2	0.24	0.12	0.24
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG21	2	0.24	0.1	0.24
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG22	2	0.24	0.1	0.24
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG23	2	0.24	0.1	0.24
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG11	2	0.24	0.06	0.24
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG12	2	0.24	0.06	0.24
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG13	2	0.24	0.06	0.24
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG11	2	0.24	0.06	0.24
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG12	2	0.24	0.06	0.24
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG13	2	0.24	0.06	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG11	2	0.24	0.06	0.24
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG12	2	0.24	0.06	0.24
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG13	2	0.24	0.06	0.24
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD11	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD12	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD13	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD11	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD12	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD13	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD11	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD12	2	0.23	0.07	0.23
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD13	2	0.23	0.07	0.23
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG21	2	0.23	0.06	0.23
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG22	2	0.23	0.06	0.23
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG23	2	0.23	0.06	0.23
(1,247)	1:223:A:GLU:H	1:225:A:GLU:H	2	0.22	0.04	0.22
(1,63)	1:96:A:ILE:H	1:97:A:GLY:H	2	0.22	0.03	0.22
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD21	2	0.21	0.11	0.21
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD22	2	0.21	0.11	0.21
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD23	2	0.21	0.11	0.21
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	2	0.2	0.06	0.2
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	2	0.2	0.06	0.2
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD11	2	0.2	0.06	0.2
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD12	2	0.2	0.06	0.2
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD13	2	0.2	0.06	0.2
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD21	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD22	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD23	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD21	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD22	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD23	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD21	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD22	2	0.2	0.1	0.2
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD23	2	0.2	0.1	0.2
(1,279)	1:134:A:PHE:H	1:137:A:GLY:H	2	0.2	0.06	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	2	0.19	0.08	0.19
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	2	0.19	0.08	0.19
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD11	2	0.19	0.06	0.19
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD12	2	0.19	0.06	0.19
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD13	2	0.19	0.06	0.19
(1,267)	1:99:A:THR:H	1:102:A:ASP:H	2	0.18	0.06	0.18
(1,336)	1:93:A:ASP:H	1:186:A:VAL:H	2	0.18	0.02	0.18
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG21	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG22	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG23	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG21	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG22	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG23	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG21	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG22	2	0.18	0.01	0.18
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG23	2	0.18	0.01	0.18
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD21	2	0.18	0.05	0.18
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD22	2	0.18	0.05	0.18
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD23	2	0.18	0.05	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	2	0.18	0.0	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	2	0.18	0.0	0.18
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB1	2	0.18	0.03	0.18
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB2	2	0.18	0.03	0.18
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB3	2	0.18	0.03	0.18
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG11	2	0.18	0.06	0.18
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG12	2	0.18	0.06	0.18
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG13	2	0.18	0.06	0.18
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG11	2	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG12	2	0.18	0.03	0.18
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG13	2	0.18	0.03	0.18
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG11	2	0.18	0.03	0.18
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG12	2	0.18	0.03	0.18
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG13	2	0.18	0.03	0.18
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG11	2	0.18	0.03	0.18
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG12	2	0.18	0.03	0.18
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG13	2	0.18	0.03	0.18
(1,342)	1:146:A:GLU:H	1:191:A:LYS:H	2	0.17	0.06	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB1	2	0.17	0.0	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB2	2	0.17	0.0	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB3	2	0.17	0.0	0.17
(1,47)	1:76:A:LEU:H	1:77:A:HIS:H	2	0.17	0.02	0.17
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG21	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG22	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG23	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG21	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG22	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG23	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG21	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG22	2	0.17	0.04	0.17
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG23	2	0.17	0.04	0.17
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD11	2	0.17	0.07	0.17
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD12	2	0.17	0.07	0.17
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD13	2	0.17	0.07	0.17
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD11	2	0.17	0.05	0.17
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD12	2	0.17	0.05	0.17
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD13	2	0.17	0.05	0.17
(1,61)	1:94:A:THR:H	1:95:A:GLY:H	2	0.16	0.01	0.16
(1,193)	1:72:A:SER:H	1:74:A:LYS:H	2	0.16	0.02	0.16
(1,325)	1:80:A:LEU:H	1:221:A:PHE:H	2	0.16	0.02	0.16
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD11	2	0.16	0.01	0.16
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD12	2	0.16	0.01	0.16
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD13	2	0.16	0.01	0.16
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	2	0.16	0.04	0.16
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	2	0.16	0.04	0.16
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	2	0.16	0.04	0.16
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	2	0.16	0.04	0.16
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	2	0.16	0.04	0.16
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	2	0.16	0.04	0.16
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	2	0.16	0.04	0.16
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	2	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	2	0.16	0.04	0.16
(1,280)	1:136:A:VAL:H	1:139:A:TYR:H	2	0.16	0.04	0.16
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	2	0.16	0.02	0.16
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	2	0.16	0.02	0.16
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD21	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD22	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD23	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD21	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD22	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD23	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD21	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD22	2	0.16	0.03	0.16
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD23	2	0.16	0.03	0.16
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	2	0.16	0.05	0.16
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	2	0.16	0.05	0.16
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD11	2	0.16	0.01	0.16
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD12	2	0.16	0.01	0.16
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD13	2	0.16	0.01	0.16
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE1	2	0.16	0.01	0.16
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE2	2	0.16	0.01	0.16
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE3	2	0.16	0.01	0.16
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB1	2	0.16	0.05	0.16
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB2	2	0.16	0.05	0.16
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB3	2	0.16	0.05	0.16
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD21	2	0.16	0.02	0.16
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD22	2	0.16	0.02	0.16
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD23	2	0.16	0.02	0.16
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD21	2	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD22	2	0.16	0.02	0.16
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD23	2	0.16	0.02	0.16
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD21	2	0.16	0.02	0.16
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD22	2	0.16	0.02	0.16
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD23	2	0.16	0.02	0.16
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD11	2	0.16	0.02	0.16
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD12	2	0.16	0.02	0.16
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD13	2	0.16	0.02	0.16
(1,221)	1:180:A:MET:H	1:182:A:ARG:H	2	0.16	0.05	0.16
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	2	0.16	0.05	0.16
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE1	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE2	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE3	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE1	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE2	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE3	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE1	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE2	2	0.16	0.04	0.16
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE3	2	0.16	0.04	0.16
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD11	2	0.16	0.05	0.16
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD12	2	0.16	0.05	0.16
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD13	2	0.16	0.05	0.16
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD11	2	0.15	0.01	0.15
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD12	2	0.15	0.01	0.15
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD13	2	0.15	0.01	0.15
(1,364)	1:225:A:GLU:H	1:230:A:VAL:H	2	0.15	0.04	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD21	2	0.15	0.0	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD22	2	0.15	0.0	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD23	2	0.15	0.0	0.15
(2,16)	1:79:A:ASN:H	1:92:A:VAL:O	2	0.15	0.04	0.15
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD11	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD12	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD13	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD11	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD12	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD13	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD11	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD12	2	0.15	0.02	0.15
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD13	2	0.15	0.02	0.15
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG11	2	0.15	0.0	0.15
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG12	2	0.15	0.0	0.15
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG13	2	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG11	2	0.15	0.0	0.15
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG12	2	0.15	0.0	0.15
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG13	2	0.15	0.0	0.15
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG11	2	0.15	0.0	0.15
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG12	2	0.15	0.0	0.15
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG13	2	0.15	0.0	0.15
(2,82)	1:28:A:GLN:H	1:24:A:ALA:O	2	0.15	0.04	0.15
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG21	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG22	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG23	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG21	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG22	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG23	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG21	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG22	2	0.14	0.03	0.14
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG23	2	0.14	0.03	0.14
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD11	2	0.14	0.01	0.14
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD12	2	0.14	0.01	0.14
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD13	2	0.14	0.01	0.14
(1,276)	1:128:A:ILE:H	1:131:A:ILE:H	2	0.14	0.01	0.14
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB1	2	0.14	0.02	0.14
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB2	2	0.14	0.02	0.14
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB3	2	0.14	0.02	0.14
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG21	2	0.14	0.01	0.14
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG22	2	0.14	0.01	0.14
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG23	2	0.14	0.01	0.14
(1,208)	1:123:A:GLN:H	1:125:A:GLY:H	2	0.13	0.01	0.13
(1,286)	1:192:A:GLU:H	1:195:A:THR:H	2	0.13	0.0	0.13
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD11	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD12	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD13	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD11	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD12	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD13	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD11	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD12	2	0.13	0.03	0.13
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD13	2	0.13	0.03	0.13
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD11	2	0.13	0.02	0.13
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD12	2	0.13	0.02	0.13
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD13	2	0.13	0.02	0.13
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG21	2	0.13	0.03	0.13
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG22	2	0.13	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG23	2	0.13	0.03	0.13
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG21	2	0.13	0.03	0.13
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG22	2	0.13	0.03	0.13
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG23	2	0.13	0.03	0.13
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB1	2	0.13	0.01	0.13
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB2	2	0.13	0.01	0.13
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB3	2	0.13	0.01	0.13
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	2	0.12	0.01	0.12
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	2	0.12	0.01	0.12
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	2	0.12	0.02	0.12
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	2	0.12	0.02	0.12
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD11	2	0.12	0.02	0.12
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD12	2	0.12	0.02	0.12
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD13	2	0.12	0.02	0.12
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD21	2	0.12	0.01	0.12
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD22	2	0.12	0.01	0.12
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD23	2	0.12	0.01	0.12
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD21	2	0.12	0.01	0.12
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD22	2	0.12	0.01	0.12
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD23	2	0.12	0.01	0.12
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD21	2	0.12	0.01	0.12
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD22	2	0.12	0.01	0.12
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD23	2	0.12	0.01	0.12
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG21	2	0.12	0.01	0.12
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG22	2	0.12	0.01	0.12
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG23	2	0.12	0.01	0.12
(1,220)	1:167:A:GLY:H	1:169:A:SER:H	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD21	2	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD22	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD23	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD21	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD22	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD23	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD21	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD22	2	0.12	0.02	0.12
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD23	2	0.12	0.02	0.12
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG11	2	0.12	0.02	0.12
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG12	2	0.12	0.02	0.12
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG13	2	0.12	0.02	0.12
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD11	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD12	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD13	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD11	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD12	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD13	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD11	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD12	2	0.12	0.0	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD13	2	0.12	0.0	0.12
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG21	2	0.12	0.01	0.12
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG22	2	0.12	0.01	0.12
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG23	2	0.12	0.01	0.12
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD11	2	0.12	0.01	0.12
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD12	2	0.12	0.01	0.12
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD13	2	0.12	0.01	0.12
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE1	2	0.12	0.01	0.12
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE2	2	0.12	0.01	0.12
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE3	2	0.12	0.01	0.12
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD21	2	0.12	0.02	0.12
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD22	2	0.12	0.02	0.12
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD23	2	0.12	0.02	0.12
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD21	2	0.12	0.02	0.12

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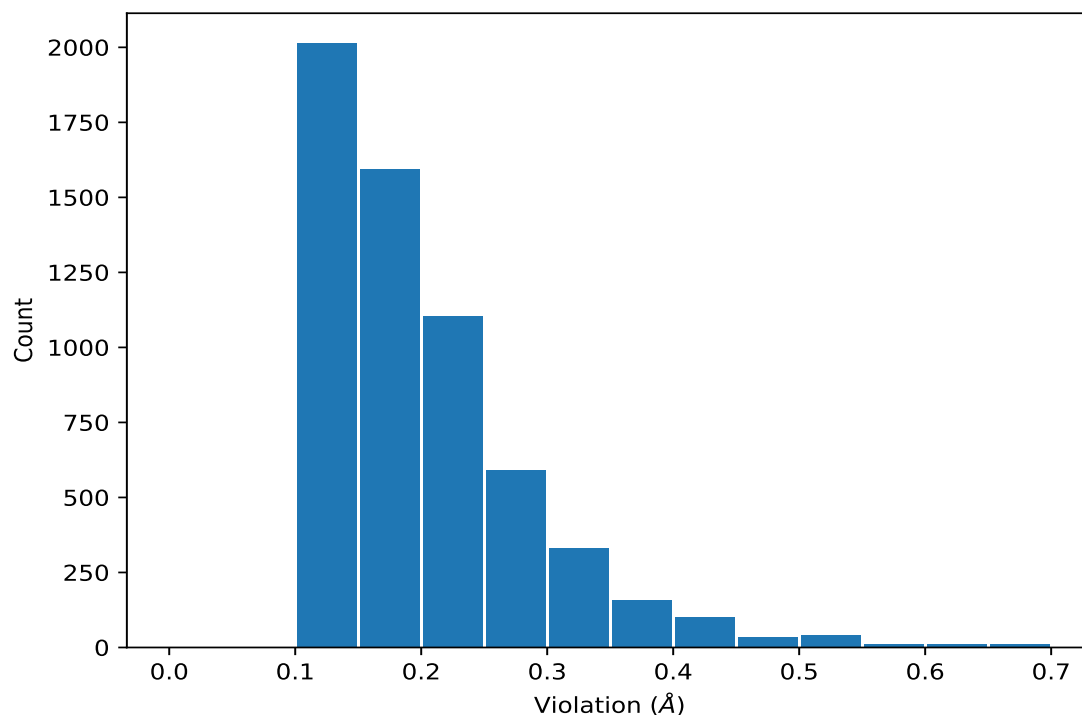
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD22	2	0.12	0.02	0.12
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD23	2	0.12	0.02	0.12
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD21	2	0.12	0.02	0.12
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD22	2	0.12	0.02	0.12
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD23	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	2	0.12	0.02	0.12
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	2	0.12	0.02	0.12
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD11	2	0.12	0.02	0.12
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD12	2	0.12	0.02	0.12
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD13	2	0.12	0.02	0.12
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG21	2	0.12	0.02	0.12
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG22	2	0.12	0.02	0.12
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG23	2	0.12	0.02	0.12
(1,218)	1:145:A:ALA:H	1:147:A:LYS:H	2	0.12	0.0	0.12
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD21	2	0.12	0.0	0.12
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD22	2	0.12	0.0	0.12
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD23	2	0.12	0.0	0.12
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD21	2	0.12	0.0	0.12
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD22	2	0.12	0.0	0.12
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD23	2	0.12	0.0	0.12
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	2	0.11	0.01	0.11
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	2	0.11	0.01	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD11	2	0.11	0.0	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD12	2	0.11	0.0	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD13	2	0.11	0.0	0.11
(2,97)	1:44:A:PHE:N	1:41:A:LYS:O	2	0.1	0.0	0.1

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)
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	10	0.7
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	10	0.7
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	10	0.7
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	10	0.7
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	10	0.7
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	10	0.7
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	10	0.7
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	10	0.7
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	10	0.7
(1,87)	1:137:A:GLY:H	1:138:A:PHE:H	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	3	0.63
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	3	0.63
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	3	0.63
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	3	0.63
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	3	0.63
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	3	0.63
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	3	0.63
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	3	0.63
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	3	0.63
(1,87)	1:137:A:GLY:H	1:138:A:PHE:H	3	0.6
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD11	5	0.55
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD12	5	0.55
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD13	5	0.55
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	4	0.55
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	4	0.55
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	4	0.55
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	4	0.55
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	4	0.55
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	4	0.55
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	4	0.55
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	4	0.55
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	4	0.55
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD11	4	0.54
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD12	4	0.54
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD13	4	0.54
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD11	4	0.54
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD12	4	0.54
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD13	4	0.54
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD11	4	0.54
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD12	4	0.54
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD13	4	0.54
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG11	8	0.52
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG12	8	0.52
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG13	8	0.52
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	1	0.52
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	1	0.52
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	1	0.52
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	1	0.52
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	1	0.52
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	1	0.52
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	1	0.52
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	1	0.52
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD11	2	0.51
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD12	2	0.51
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD13	2	0.51
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	7	0.51
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	7	0.51
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	7	0.51
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	7	0.51
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	7	0.51
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	7	0.51
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	7	0.51
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	7	0.51
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	7	0.51
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	2	0.51
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	2	0.51
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	2	0.51
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	2	0.51
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	2	0.51
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	2	0.51
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	2	0.51
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	2	0.51
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	2	0.51
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	8	0.5
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG21	3	0.49
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG22	3	0.49
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG23	3	0.49
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	1	0.49
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	1	0.49
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	1	0.49
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	1	0.49
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	1	0.49
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	1	0.49
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	1	0.49
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	1	0.49
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	1	0.49
(1,219)	1:164:A:SER:H	1:166:A:ALA:H	1	0.49
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	7	0.46
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	7	0.46
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	7	0.46
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	2	0.46
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	2	0.46
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	2	0.46
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	2	0.46
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	2	0.46
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	2	0.46
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	2	0.46
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	2	0.46
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	4	0.45
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	4	0.45
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	4	0.45
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	4	0.45
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	4	0.45
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	4	0.45
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	4	0.45
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	4	0.45
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	4	0.45
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	7	0.45
(1,1099)	1:223:A:GLU:H	1:222:A:VAL:HG21	5	0.44
(1,1099)	1:223:A:GLU:H	1:222:A:VAL:HG22	5	0.44
(1,1099)	1:223:A:GLU:H	1:222:A:VAL:HG23	5	0.44
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG21	4	0.44
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG22	4	0.44
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG23	4	0.44
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG21	10	0.44
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG22	10	0.44
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG23	10	0.44
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	4	0.44
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	4	0.44
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	4	0.44
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	4	0.44
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	4	0.44
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	4	0.44
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	4	0.44
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	4	0.44
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	4	0.44
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	10	0.43
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	10	0.43
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	10	0.43
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	10	0.43
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	10	0.43
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	10	0.43
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	10	0.43
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	10	0.43
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	7	0.42
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	7	0.42
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	7	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	7	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	7	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	7	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	7	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	7	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	7	0.42
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	9	0.42
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	9	0.42
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	9	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	9	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	9	0.42
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	9	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	9	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	9	0.42
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	9	0.42
(1,108)	1:166:A:ALA:H	1:167:A:GLY:H	6	0.42
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD11	7	0.41
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD12	7	0.41
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD13	7	0.41
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG11	5	0.41
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG12	5	0.41
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG13	5	0.41
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	3	0.41
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	3	0.41
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	3	0.41
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	4	0.41
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	4	0.41
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	4	0.41
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB1	3	0.41
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB2	3	0.41
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB3	3	0.41
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	2	0.41
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	2	0.41
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	2	0.41
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	2	0.41
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	2	0.41
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	2	0.41
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	2	0.41
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	2	0.41
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	5	0.41
(1,287)	1:194:A:GLN:H	1:197:A:TYR:H	1	0.41
(1,108)	1:166:A:ALA:H	1:167:A:GLY:H	9	0.41
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG11	8	0.4
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG12	8	0.4
(1,972)	1:173:A:ARG:H	1:172:A:VAL:HG13	8	0.4
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB1	4	0.4
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB2	4	0.4
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB3	4	0.4
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG11	5	0.4
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG12	5	0.4
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG13	5	0.4
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	3	0.4
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	3	0.4
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	3	0.4
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	3	0.4
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	3	0.4
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	3	0.4
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	3	0.4
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	3	0.4
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	3	0.4
(1,480)	1:80:A:LEU:HD11	1:207:A:VAL:HG11	4	0.4
(1,480)	1:80:A:LEU:HD11	1:207:A:VAL:HG12	4	0.4
(1,480)	1:80:A:LEU:HD11	1:207:A:VAL:HG13	4	0.4
(1,480)	1:80:A:LEU:HD12	1:207:A:VAL:HG11	4	0.4
(1,480)	1:80:A:LEU:HD12	1:207:A:VAL:HG12	4	0.4
(1,480)	1:80:A:LEU:HD12	1:207:A:VAL:HG13	4	0.4
(1,480)	1:80:A:LEU:HD13	1:207:A:VAL:HG11	4	0.4
(1,480)	1:80:A:LEU:HD13	1:207:A:VAL:HG12	4	0.4
(1,480)	1:80:A:LEU:HD13	1:207:A:VAL:HG13	4	0.4
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	6	0.4
(1,116)	1:176:A:THR:H	1:177:A:GLY:H	6	0.4
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD21	3	0.39
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD22	3	0.39
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD23	3	0.39
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	2	0.39
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	2	0.39
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	2	0.39
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	5	0.39
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	5	0.39
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	5	0.39
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	5	0.39
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	5	0.39
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	5	0.39
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	5	0.39
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	5	0.39
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	3	0.39
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	3	0.39
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	3	0.39
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	3	0.39
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	3	0.39
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	3	0.39
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	3	0.39
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	3	0.39
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	3	0.39
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	5	0.39
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	5	0.39
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	5	0.39
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	5	0.39
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	5	0.39
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	5	0.39
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	5	0.39
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	5	0.39
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	5	0.39
(1,312)	1:55:A:ALA:H	1:96:A:ILE:H	7	0.39
(1,70)	1:106:A:ASN:H	1:107:A:LEU:H	5	0.39
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	7	0.38
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	7	0.38
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	7	0.38
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	7	0.38
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	7	0.38
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	7	0.38
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	7	0.38
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	7	0.38
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	7	0.38
(1,101)	1:158:A:GLU:H	1:159:A:GLN:H	9	0.38
(2,70)	1:183:A:GLY:H	1:153:A:LYS:O	1	0.37
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG21	8	0.37
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG22	8	0.37
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG23	8	0.37
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	3	0.37
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	3	0.37
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG12	2	0.37
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG13	2	0.37
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	7	0.37
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	7	0.37
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	7	0.37
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	7	0.37
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	7	0.37
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	7	0.37
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	7	0.37
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	7	0.37
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	7	0.37
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG11	5	0.37
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG12	5	0.37
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG13	5	0.37
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG11	5	0.37
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG12	5	0.37
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG13	5	0.37
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG11	5	0.37
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG12	5	0.37
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG13	5	0.37
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	3	0.37
(1,131)	1:195:A:THR:H	1:196:A:GLU:H	5	0.37
(1,109)	1:167:A:GLY:H	1:168:A:GLY:H	6	0.37
(1,45)	1:74:A:LYS:H	1:75:A:GLU:H	2	0.37
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	7	0.36
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	7	0.36
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	7	0.36
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG21	2	0.36
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG22	2	0.36
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG23	2	0.36
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	4	0.36
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	4	0.36
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	4	0.36
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	9	0.36
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	9	0.36
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	9	0.36
(1,798)	1:83:A:ASN:H	1:88:A:THR:HG21	2	0.36
(1,798)	1:83:A:ASN:H	1:88:A:THR:HG22	2	0.36
(1,798)	1:83:A:ASN:H	1:88:A:THR:HG23	2	0.36
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG12	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG13	5	0.36
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG21	3	0.36
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG22	3	0.36
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG23	3	0.36
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG21	3	0.36
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG22	3	0.36
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG23	3	0.36
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG21	3	0.36
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG22	3	0.36
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG23	3	0.36
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	5	0.36
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	5	0.36
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	5	0.36
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	5	0.36
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	5	0.36
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	5	0.36
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	5	0.36
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	5	0.36
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	5	0.36
(1,356)	1:159:A:GLN:H	1:175:A:ASP:H	5	0.36
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG11	5	0.35
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG12	5	0.35
(1,946)	1:161:A:ALA:H	1:172:A:VAL:HG13	5	0.35
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	3	0.35
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	3	0.35
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	3	0.35
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	6	0.35
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	6	0.35
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	6	0.35
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB1	2	0.35
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB2	2	0.35
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB3	2	0.35
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG12	7	0.35
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG13	7	0.35
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD11	9	0.35
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD12	9	0.35
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD13	9	0.35
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	10	0.35
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	10	0.35
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	10	0.35
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	10	0.35
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	10	0.35
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	10	0.35
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	10	0.35
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	10	0.35
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	4	0.35
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	4	0.35
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	4	0.35
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	4	0.35
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	4	0.35
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	4	0.35
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	4	0.35
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	4	0.35
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	4	0.35
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	4	0.35
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	4	0.35
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	4	0.35
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	4	0.35
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	4	0.35
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	4	0.35
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	4	0.35
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	4	0.35
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	4	0.35
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	2	0.35
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD11	8	0.34
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD12	8	0.34
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD13	8	0.34
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD11	4	0.34
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD12	4	0.34
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD13	4	0.34
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	2	0.34
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	2	0.34
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	2	0.34
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	9	0.34
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	9	0.34
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	9	0.34
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	2	0.34
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	2	0.34
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	2	0.34
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB1	3	0.34
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB2	3	0.34
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB3	3	0.34
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB1	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB2	3	0.34
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB3	3	0.34
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB1	3	0.34
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB2	3	0.34
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB3	3	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	6	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	6	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	6	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	6	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	6	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	6	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	6	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	6	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	6	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	9	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	9	0.34
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	9	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	9	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	9	0.34
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	9	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	9	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	9	0.34
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	9	0.34
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	7	0.34
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	7	0.34
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	7	0.34
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	7	0.34
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	7	0.34
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	7	0.34
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	7	0.34
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	7	0.34
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	7	0.34
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	3	0.34
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	3	0.34
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	3	0.34
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	3	0.34
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	3	0.34
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	3	0.34
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	3	0.34
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	3	0.34
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	3	0.34
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	3	0.34
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	3	0.34
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	3	0.34
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	3	0.34
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	3	0.34
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	3	0.34
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	3	0.34
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	3	0.34
(1,118)	1:181:A:GLY:H	1:182:A:ARG:H	8	0.34
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD11	4	0.33
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD12	4	0.33
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD13	4	0.33
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG21	5	0.33
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG22	5	0.33
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG23	5	0.33
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB1	8	0.33
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB2	8	0.33
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB3	8	0.33
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	8	0.33
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	8	0.33
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	8	0.33
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	1	0.33
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	1	0.33
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	1	0.33
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG21	1	0.33
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG22	1	0.33
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG23	1	0.33
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	5	0.33
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	5	0.33
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	5	0.33
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	5	0.33
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	5	0.33
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	5	0.33
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	5	0.33
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	5	0.33
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	5	0.33
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	2	0.33
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	2	0.33
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	2	0.33
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	2	0.33
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	2	0.33
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	2	0.33
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	2	0.33
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	2	0.33
(1,281)	1:138:A:PHE:H	1:141:A:ALA:H	2	0.33
(1,209)	1:124:A:ALA:H	1:126:A:ALA:H	6	0.33
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD11	1	0.32
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD12	1	0.32
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD13	1	0.32
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	8	0.32
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	8	0.32
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	8	0.32
(1,762)	1:69:A:LYS:H	1:70:A:LEU:HD11	9	0.32
(1,762)	1:69:A:LYS:H	1:70:A:LEU:HD12	9	0.32
(1,762)	1:69:A:LYS:H	1:70:A:LEU:HD13	9	0.32
(1,753)	1:62:A:GLU:H	1:59:A:ILE:HD11	3	0.32
(1,753)	1:62:A:GLU:H	1:59:A:ILE:HD12	3	0.32
(1,753)	1:62:A:GLU:H	1:59:A:ILE:HD13	3	0.32
(1,693)	1:31:A:SER:H	1:30:A:MET:HE1	4	0.32
(1,693)	1:31:A:SER:H	1:30:A:MET:HE2	4	0.32
(1,693)	1:31:A:SER:H	1:30:A:MET:HE3	4	0.32
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG21	4	0.32
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG22	4	0.32
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG23	4	0.32
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD21	10	0.32
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD22	10	0.32
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD23	10	0.32
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	8	0.32
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	8	0.32
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	8	0.32
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	8	0.32
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	8	0.32
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	8	0.32
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	8	0.32
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	8	0.32
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	8	0.32
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	4	0.32
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	4	0.32
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	4	0.32
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	4	0.32
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	4	0.32
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	4	0.32
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	4	0.32
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	4	0.32
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	8	0.32
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	8	0.32
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	8	0.32
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	8	0.32
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	8	0.32
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	8	0.32
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	8	0.32
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	8	0.32
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	8	0.32
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	10	0.32
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	10	0.32
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	10	0.32
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	10	0.32
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	10	0.32
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	10	0.32
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	10	0.32
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	10	0.32
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	10	0.32
(1,1035)	1:197:A:TYR:H	1:195:A:THR:HG21	1	0.31
(1,1035)	1:197:A:TYR:H	1:195:A:THR:HG22	1	0.31
(1,1035)	1:197:A:TYR:H	1:195:A:THR:HG23	1	0.31
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	2	0.31
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	2	0.31
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	2	0.31
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	5	0.31
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	5	0.31
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	5	0.31
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG21	7	0.31
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG22	7	0.31
(1,959)	1:163:A:GLU:H	1:171:A:THR:HG23	7	0.31
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	10	0.31
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	10	0.31
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	10	0.31
(1,929)	1:150:A:VAL:H	1:151:A:ILE:HD11	5	0.31
(1,929)	1:150:A:VAL:H	1:151:A:ILE:HD12	5	0.31
(1,929)	1:150:A:VAL:H	1:151:A:ILE:HD13	5	0.31
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD21	3	0.31
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD22	3	0.31
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD23	3	0.31
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	6	0.31
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	6	0.31
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG12	3	0.31
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG13	3	0.31
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	4	0.31
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	4	0.31
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	4	0.31
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	4	0.31
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	4	0.31
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	4	0.31
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	4	0.31
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	4	0.31
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	4	0.31
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	8	0.31
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	8	0.31
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	8	0.31
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	8	0.31
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	8	0.31
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	8	0.31
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	8	0.31
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	8	0.31
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	8	0.31
(1,426)	1:33:A:ILE:HD11	1:131:A:ILE:HD11	5	0.31
(1,426)	1:33:A:ILE:HD11	1:131:A:ILE:HD12	5	0.31
(1,426)	1:33:A:ILE:HD11	1:131:A:ILE:HD13	5	0.31
(1,426)	1:33:A:ILE:HD12	1:131:A:ILE:HD11	5	0.31
(1,426)	1:33:A:ILE:HD12	1:131:A:ILE:HD12	5	0.31
(1,426)	1:33:A:ILE:HD12	1:131:A:ILE:HD13	5	0.31
(1,426)	1:33:A:ILE:HD13	1:131:A:ILE:HD11	5	0.31
(1,426)	1:33:A:ILE:HD13	1:131:A:ILE:HD12	5	0.31
(1,426)	1:33:A:ILE:HD13	1:131:A:ILE:HD13	5	0.31
(1,337)	1:103:A:LEU:H	1:107:A:LEU:H	4	0.31
(1,281)	1:138:A:PHE:H	1:141:A:ALA:H	9	0.31
(1,277)	1:131:A:ILE:H	1:134:A:PHE:H	5	0.31
(1,87)	1:137:A:GLY:H	1:138:A:PHE:H	2	0.31
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD21	6	0.3
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD22	6	0.3
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD23	6	0.3
(1,906)	1:142:A:TYR:H	1:148:A:VAL:HG11	3	0.3
(1,906)	1:142:A:TYR:H	1:148:A:VAL:HG12	3	0.3
(1,906)	1:142:A:TYR:H	1:148:A:VAL:HG13	3	0.3
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG21	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG22	6	0.3
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG23	6	0.3
(1,885)	1:134:A:PHE:H	1:136:A:VAL:HG21	5	0.3
(1,885)	1:134:A:PHE:H	1:136:A:VAL:HG22	5	0.3
(1,885)	1:134:A:PHE:H	1:136:A:VAL:HG23	5	0.3
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB1	3	0.3
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB2	3	0.3
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB3	3	0.3
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD11	1	0.3
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD12	1	0.3
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD13	1	0.3
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB1	3	0.3
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB2	3	0.3
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB3	3	0.3
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG21	3	0.3
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG22	3	0.3
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG23	3	0.3
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG21	7	0.3
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG22	7	0.3
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG23	7	0.3
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD11	7	0.3
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD12	7	0.3
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD13	7	0.3
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD11	7	0.3
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD12	7	0.3
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD13	7	0.3
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD11	7	0.3
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD12	7	0.3
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD13	7	0.3
(1,587)	1:195:A:THR:HG21	1:198:A:LEU:HD21	3	0.3
(1,587)	1:195:A:THR:HG21	1:198:A:LEU:HD22	3	0.3
(1,587)	1:195:A:THR:HG21	1:198:A:LEU:HD23	3	0.3
(1,587)	1:195:A:THR:HG22	1:198:A:LEU:HD21	3	0.3
(1,587)	1:195:A:THR:HG22	1:198:A:LEU:HD22	3	0.3
(1,587)	1:195:A:THR:HG22	1:198:A:LEU:HD23	3	0.3
(1,587)	1:195:A:THR:HG23	1:198:A:LEU:HD21	3	0.3
(1,587)	1:195:A:THR:HG23	1:198:A:LEU:HD22	3	0.3
(1,587)	1:195:A:THR:HG23	1:198:A:LEU:HD23	3	0.3
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	6	0.3
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	6	0.3
(1,567)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	6	0.3
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	6	0.3
(1,567)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	6	0.3
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	6	0.3
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	6	0.3
(1,567)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	6	0.3
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD21	3	0.3
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD22	3	0.3
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD23	3	0.3
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD21	3	0.3
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD22	3	0.3
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD23	3	0.3
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD21	3	0.3
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD22	3	0.3
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD23	3	0.3
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG21	10	0.3
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG22	10	0.3
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG23	10	0.3
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG21	10	0.3
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG22	10	0.3
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG23	10	0.3
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG21	10	0.3
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG22	10	0.3
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG23	10	0.3
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	10	0.3
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	10	0.3
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	10	0.3
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	10	0.3
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	10	0.3
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	10	0.3
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	10	0.3
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	10	0.3
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	10	0.3
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	2	0.3
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	2	0.3
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	2	0.3
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	2	0.3
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	2	0.3
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	2	0.3
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	2	0.3
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	2	0.3
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	2	0.3
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	10	0.3
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	10	0.3
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	10	0.3
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	10	0.3
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	10	0.3
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	10	0.3
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	10	0.3
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	10	0.3
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG11	5	0.3
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG12	5	0.3
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG13	5	0.3
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG11	5	0.3
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG12	5	0.3
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG13	5	0.3
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG11	5	0.3
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG12	5	0.3
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG13	5	0.3
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD11	4	0.29
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD12	4	0.29
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD13	4	0.29
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG21	6	0.29
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG22	6	0.29
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG23	6	0.29
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD11	1	0.29
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD12	1	0.29
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD13	1	0.29
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG21	10	0.29
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG22	10	0.29
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG23	10	0.29
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	1	0.29
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	1	0.29
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	1	0.29
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	10	0.29
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	10	0.29
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	10	0.29
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	4	0.29
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	4	0.29
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	4	0.29
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	7	0.29
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	7	0.29
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	7	0.29
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	10	0.29
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	10	0.29
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	4	0.29
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	4	0.29
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	4	0.29
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	10	0.29
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	10	0.29
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	10	0.29
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG21	2	0.29
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG22	2	0.29
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG23	2	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD11	6	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD12	6	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD13	6	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD11	7	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD12	7	0.29
(1,599)	1:26:A:ILE:H	1:26:A:ILE:HD13	7	0.29
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG21	3	0.29
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG22	3	0.29
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG23	3	0.29
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	2	0.29
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	2	0.29
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	2	0.29
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	2	0.29
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	2	0.29
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	2	0.29
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	2	0.29
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	2	0.29
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	2	0.29
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	9	0.29
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	9	0.29
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	9	0.29
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	9	0.29
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	9	0.29
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	9	0.29
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	9	0.29
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	9	0.29
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	9	0.29
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	4	0.29
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	4	0.29
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	4	0.29
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	4	0.29
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	4	0.29
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	4	0.29
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	4	0.29
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	4	0.29
(1,506)	1:92:A:VAL:HG21	1:94:A:THR:HG21	8	0.29
(1,506)	1:92:A:VAL:HG21	1:94:A:THR:HG22	8	0.29
(1,506)	1:92:A:VAL:HG21	1:94:A:THR:HG23	8	0.29
(1,506)	1:92:A:VAL:HG22	1:94:A:THR:HG21	8	0.29
(1,506)	1:92:A:VAL:HG22	1:94:A:THR:HG22	8	0.29
(1,506)	1:92:A:VAL:HG22	1:94:A:THR:HG23	8	0.29
(1,506)	1:92:A:VAL:HG23	1:94:A:THR:HG21	8	0.29
(1,506)	1:92:A:VAL:HG23	1:94:A:THR:HG22	8	0.29
(1,506)	1:92:A:VAL:HG23	1:94:A:THR:HG23	8	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	1	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	1	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	1	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	1	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	1	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	1	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	1	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	1	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	1	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	6	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	6	0.29
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	6	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	6	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	6	0.29
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	6	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	6	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	6	0.29
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	6	0.29
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	9	0.29
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	9	0.29
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	9	0.29
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	9	0.29
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	9	0.29
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	9	0.29
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	9	0.29
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	9	0.29
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	9	0.29
(1,337)	1:103:A:LEU:H	1:107:A:LEU:H	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:60:A:ARG:H	1:96:A:ILE:H	2	0.29
(1,46)	1:75:A:GLU:H	1:76:A:LEU:H	6	0.29
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	4	0.28
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	4	0.28
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	4	0.28
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG21	5	0.28
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG22	5	0.28
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG23	5	0.28
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG11	5	0.28
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG12	5	0.28
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG13	5	0.28
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	9	0.28
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	9	0.28
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	9	0.28
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	6	0.28
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	6	0.28
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	6	0.28
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	10	0.28
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	10	0.28
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	10	0.28
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD11	2	0.28
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD12	2	0.28
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD13	2	0.28
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB1	8	0.28
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB2	8	0.28
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB3	8	0.28
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	5	0.28
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	5	0.28
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	5	0.28
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	3	0.28
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	3	0.28
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	3	0.28
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	2	0.28
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	2	0.28
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	2	0.28
(1,681)	1:22:A:PHE:H	1:21:A:ALA:HB1	7	0.28
(1,681)	1:22:A:PHE:H	1:21:A:ALA:HB2	7	0.28
(1,681)	1:22:A:PHE:H	1:21:A:ALA:HB3	7	0.28
(1,632)	1:107:A:LEU:H	1:107:A:LEU:HD11	6	0.28
(1,632)	1:107:A:LEU:H	1:107:A:LEU:HD12	6	0.28
(1,632)	1:107:A:LEU:H	1:107:A:LEU:HD13	6	0.28
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	5	0.28
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	5	0.28
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	5	0.28
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	5	0.28
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	5	0.28
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	5	0.28
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	5	0.28
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	5	0.28
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	1	0.28
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	1	0.28
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	1	0.28
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	1	0.28
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	1	0.28
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	1	0.28
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	1	0.28
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	1	0.28
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	1	0.28
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB1	1	0.28
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB2	1	0.28
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB3	1	0.28
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB1	1	0.28
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB2	1	0.28
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB3	1	0.28
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB1	1	0.28
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB2	1	0.28
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB3	1	0.28
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG21	2	0.28
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG22	2	0.28
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG23	2	0.28
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG21	2	0.28
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG22	2	0.28
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG23	2	0.28
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG21	2	0.28
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG22	2	0.28
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG23	2	0.28
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	2	0.28
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	2	0.28
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	2	0.28
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	2	0.28
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	2	0.28
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	2	0.28
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	2	0.28
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	2	0.28
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	3	0.28
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	3	0.28
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	3	0.28
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	3	0.28
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	3	0.28
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	3	0.28
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	3	0.28
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	3	0.28
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	3	0.28
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD11	5	0.28
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD12	5	0.28
(1,450)	1:45:A:LEU:HD21	1:206:A:ILE:HD13	5	0.28
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD11	5	0.28
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD12	5	0.28
(1,450)	1:45:A:LEU:HD22	1:206:A:ILE:HD13	5	0.28
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD11	5	0.28
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD12	5	0.28
(1,450)	1:45:A:LEU:HD23	1:206:A:ILE:HD13	5	0.28
(1,118)	1:181:A:GLY:H	1:182:A:ARG:H	4	0.28
(1,17)	1:41:A:LYS:H	1:42:A:GLU:H	1	0.28
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD11	4	0.27
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD12	4	0.27
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD13	4	0.27
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	6	0.27
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	6	0.27
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	6	0.27
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	5	0.27
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	5	0.27
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	5	0.27
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	2	0.27
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	2	0.27
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	2	0.27
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	2	0.27
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	2	0.27
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	2	0.27
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD11	2	0.27
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD12	2	0.27
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD13	2	0.27
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	9	0.27
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	9	0.27
(1,782)	1:79:A:ASN:H	1:81:A:ILE:HD11	3	0.27
(1,782)	1:79:A:ASN:H	1:81:A:ILE:HD12	3	0.27
(1,782)	1:79:A:ASN:H	1:81:A:ILE:HD13	3	0.27
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG21	1	0.27
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG22	1	0.27
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG23	1	0.27
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	8	0.27
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	8	0.27
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	8	0.27
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	3	0.27
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	3	0.27
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	3	0.27
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	3	0.27
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	3	0.27
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	3	0.27
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	3	0.27
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	3	0.27
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	3	0.27
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	5	0.27
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	5	0.27
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	5	0.27
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	5	0.27
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	5	0.27
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	5	0.27
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	5	0.27
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	5	0.27
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	5	0.27
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB1	8	0.27
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB2	8	0.27
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB3	8	0.27
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB1	8	0.27
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB2	8	0.27
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB3	8	0.27
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB1	8	0.27
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB2	8	0.27
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB3	8	0.27
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	8	0.27
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	8	0.27
(1,501)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	8	0.27
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	8	0.27
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	8	0.27
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	8	0.27
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	8	0.27
(1,501)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	8	0.27
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	8	0.27
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	8	0.27
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	8	0.27
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	8	0.27
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	8	0.27
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	8	0.27
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	8	0.27
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	8	0.27
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	8	0.27
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	4	0.27
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	4	0.27
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	4	0.27
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	4	0.27
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	4	0.27
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	4	0.27
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	4	0.27
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	4	0.27
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	4	0.27
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	6	0.27
(1,79)	1:126:A:ALA:H	1:127:A:ASP:H	7	0.27
(1,69)	1:105:A:ASN:H	1:106:A:ASN:H	4	0.27
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	4	0.26
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	4	0.26
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	4	0.26
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD21	8	0.26
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD22	8	0.26
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD23	8	0.26
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	2	0.26
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	2	0.26
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	2	0.26
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	7	0.26
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	7	0.26
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	7	0.26
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG21	4	0.26
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG22	4	0.26
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG23	4	0.26
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB1	10	0.26
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB2	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB3	10	0.26
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD11	2	0.26
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD12	2	0.26
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD13	2	0.26
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB1	9	0.26
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB2	9	0.26
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB3	9	0.26
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	4	0.26
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	4	0.26
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	4	0.26
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	7	0.26
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	7	0.26
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	7	0.26
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD11	2	0.26
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD12	2	0.26
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD13	2	0.26
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	4	0.26
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	4	0.26
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	4	0.26
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	7	0.26
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	7	0.26
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	7	0.26
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	4	0.26
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	4	0.26
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	4	0.26
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	4	0.26
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	4	0.26
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	4	0.26
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	4	0.26
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	4	0.26
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	4	0.26
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	6	0.26
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	6	0.26
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	6	0.26
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	6	0.26
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	6	0.26
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	6	0.26
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	6	0.26
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	6	0.26
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	6	0.26
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	4	0.26
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	4	0.26
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	4	0.26
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	4	0.26
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	4	0.26
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	4	0.26
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	4	0.26
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	4	0.26
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	5	0.26
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	5	0.26
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	5	0.26
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	5	0.26
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	5	0.26
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	5	0.26
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	5	0.26
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	5	0.26
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	5	0.26
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	9	0.26
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	9	0.26
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	9	0.26
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	9	0.26
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	9	0.26
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	9	0.26
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	9	0.26
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	9	0.26
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	9	0.26
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	1	0.26
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	1	0.26
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	1	0.26
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	1	0.26
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	1	0.26
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	1	0.26
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	1	0.26
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	1	0.26
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	1	0.26
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	3	0.26
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	3	0.26
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	3	0.26
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	3	0.26
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	3	0.26
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	3	0.26
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	3	0.26
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	3	0.26
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	5	0.26
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	5	0.26
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	5	0.26
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	5	0.26
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	5	0.26
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	5	0.26
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	5	0.26
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	5	0.26
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	5	0.26
(1,312)	1:55:A:ALA:H	1:96:A:ILE:H	2	0.26
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	6	0.26
(1,279)	1:134:A:PHE:H	1:137:A:GLY:H	6	0.26
(1,247)	1:223:A:GLU:H	1:225:A:GLU:H	1	0.26
(1,202)	1:114:A:GLY:H	1:116:A:LYS:H	6	0.26
(1,101)	1:158:A:GLU:H	1:159:A:GLN:H	10	0.26
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG21	6	0.25
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG22	6	0.25
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG23	6	0.25
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	7	0.25
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	7	0.25
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	7	0.25
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD11	4	0.25
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD12	4	0.25
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD13	4	0.25
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD21	9	0.25
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD22	9	0.25
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD23	9	0.25
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	9	0.25
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	9	0.25
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	9	0.25
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	1	0.25
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	1	0.25
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	1	0.25
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG21	5	0.25
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG22	5	0.25
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG23	5	0.25
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	9	0.25
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	9	0.25
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	9	0.25
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB1	1	0.25
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB2	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB3	1	0.25
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD11	8	0.25
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD12	8	0.25
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD13	8	0.25
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	10	0.25
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	10	0.25
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	10	0.25
(1,811)	1:87:A:ARG:H	1:198:A:LEU:HD11	3	0.25
(1,811)	1:87:A:ARG:H	1:198:A:LEU:HD12	3	0.25
(1,811)	1:87:A:ARG:H	1:198:A:LEU:HD13	3	0.25
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	2	0.25
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	2	0.25
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	2	0.25
(1,773)	1:77:A:HIS:H	1:56:A:LEU:HD11	1	0.25
(1,773)	1:77:A:HIS:H	1:56:A:LEU:HD12	1	0.25
(1,773)	1:77:A:HIS:H	1:56:A:LEU:HD13	1	0.25
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	7	0.25
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	7	0.25
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	7	0.25
(1,693)	1:31:A:SER:H	1:30:A:MET:HE1	9	0.25
(1,693)	1:31:A:SER:H	1:30:A:MET:HE2	9	0.25
(1,693)	1:31:A:SER:H	1:30:A:MET:HE3	9	0.25
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	2	0.25
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	2	0.25
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	2	0.25
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD11	3	0.25
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD12	3	0.25
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD13	3	0.25
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD11	3	0.25
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD12	3	0.25
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD13	3	0.25
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD11	3	0.25
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD12	3	0.25
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD13	3	0.25
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG21	4	0.25
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG22	4	0.25
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG23	4	0.25
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG21	4	0.25
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG22	4	0.25
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG23	4	0.25
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG21	4	0.25
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG22	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG23	4	0.25
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	8	0.25
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	8	0.25
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	8	0.25
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	8	0.25
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	8	0.25
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	8	0.25
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	8	0.25
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	8	0.25
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	8	0.25
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	3	0.25
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	3	0.25
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	3	0.25
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	3	0.25
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	3	0.25
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	3	0.25
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	3	0.25
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	3	0.25
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	3	0.25
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG21	10	0.25
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG22	10	0.25
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG23	10	0.25
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG21	10	0.25
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG22	10	0.25
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG23	10	0.25
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG21	10	0.25
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG22	10	0.25
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG23	10	0.25
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	4	0.25
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	4	0.25
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	4	0.25
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	4	0.25
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	4	0.25
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	4	0.25
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	4	0.25
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	4	0.25
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	4	0.25
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	10	0.25
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	10	0.25
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	10	0.25
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	10	0.25
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	10	0.25
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	10	0.25
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	10	0.25
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	10	0.25
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	6	0.25
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	6	0.25
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	6	0.25
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	6	0.25
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	6	0.25
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	6	0.25
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	6	0.25
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	6	0.25
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	6	0.25
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	5	0.25
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	5	0.25
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	5	0.25
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	5	0.25
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	5	0.25
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	5	0.25
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	5	0.25
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	5	0.25
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	5	0.25
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	10	0.25
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	10	0.25
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	10	0.25
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	10	0.25
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	10	0.25
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	10	0.25
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	10	0.25
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	10	0.25
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	10	0.25
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	5	0.25
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	5	0.25
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	5	0.25
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	5	0.25
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	5	0.25
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	5	0.25
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	5	0.25
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	5	0.25
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	5	0.25
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB1	10	0.25
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB2	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB3	10	0.25
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB1	10	0.25
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB2	10	0.25
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB3	10	0.25
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB1	10	0.25
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB2	10	0.25
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB3	10	0.25
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	5	0.25
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	5	0.25
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	5	0.25
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	5	0.25
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	5	0.25
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	5	0.25
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	5	0.25
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	5	0.25
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	5	0.25
(1,268)	1:101:A:ALA:H	1:104:A:ILE:H	4	0.25
(1,267)	1:99:A:THR:H	1:102:A:ASP:H	3	0.25
(1,63)	1:96:A:ILE:H	1:97:A:GLY:H	10	0.25
(2,66)	1:160:A:TYR:H	1:152:A:THR:O	1	0.24
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG11	7	0.24
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG12	7	0.24
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG13	7	0.24
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	2	0.24
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	2	0.24
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	2	0.24
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD21	2	0.24
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD22	2	0.24
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD23	2	0.24
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG21	10	0.24
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG22	10	0.24
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG23	10	0.24
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG11	3	0.24
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG12	3	0.24
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG13	3	0.24
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	3	0.24
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	3	0.24
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	3	0.24
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	3	0.24
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	3	0.24
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	3	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	3	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	3	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	8	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	8	0.24
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	8	0.24
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	1	0.24
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	1	0.24
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	1	0.24
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	5	0.24
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	5	0.24
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	5	0.24
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD11	7	0.24
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD12	7	0.24
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD13	7	0.24
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG11	1	0.24
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG12	1	0.24
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG13	1	0.24
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB1	5	0.24
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB2	5	0.24
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB3	5	0.24
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD11	8	0.24
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD12	8	0.24
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD13	8	0.24
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	9	0.24
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	9	0.24
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	9	0.24
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	4	0.24
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	4	0.24
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	4	0.24
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG21	1	0.24
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG22	1	0.24
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG23	1	0.24
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD11	7	0.24
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD12	7	0.24
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD13	7	0.24
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	2	0.24
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	2	0.24
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	2	0.24
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG11	1	0.24
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG12	1	0.24
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG13	1	0.24
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	5	0.24
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	5	0.24
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	6	0.24
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	6	0.24
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	6	0.24
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	4	0.24
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	4	0.24
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	4	0.24
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG21	4	0.24
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG22	4	0.24
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG23	4	0.24
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	9	0.24
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	9	0.24
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	9	0.24
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	9	0.24
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	9	0.24
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	9	0.24
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG12	10	0.24
(1,606)	1:43:A:ILE:H	1:43:A:ILE:HG13	10	0.24
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	7	0.24
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	7	0.24
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	7	0.24
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	7	0.24
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	7	0.24
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	7	0.24
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	7	0.24
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	7	0.24
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	7	0.24
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	8	0.24
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	8	0.24
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	8	0.24
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	8	0.24
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	8	0.24
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	8	0.24
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	8	0.24
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	8	0.24
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	8	0.24
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE1	2	0.24
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE2	2	0.24
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE3	2	0.24
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE1	2	0.24
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE2	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE3	2	0.24
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE1	2	0.24
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE2	2	0.24
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE3	2	0.24
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	4	0.24
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	4	0.24
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	4	0.24
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	4	0.24
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	4	0.24
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	4	0.24
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	4	0.24
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	4	0.24
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	4	0.24
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	2	0.24
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	2	0.24
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	2	0.24
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	2	0.24
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	2	0.24
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	2	0.24
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	2	0.24
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	2	0.24
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	2	0.24
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG21	3	0.24
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG22	3	0.24
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG23	3	0.24
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG21	3	0.24
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG22	3	0.24
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG23	3	0.24
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG21	3	0.24
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG22	3	0.24
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG23	3	0.24
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	6	0.24
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	6	0.24
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	6	0.24
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	6	0.24
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	6	0.24
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	6	0.24
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	6	0.24
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	6	0.24
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	6	0.24
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	9	0.24
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	9	0.24
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	9	0.24
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	9	0.24
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	9	0.24
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	9	0.24
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	9	0.24
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	9	0.24
(1,288)	1:196:A:GLU:H	1:199:A:GLU:H	7	0.24
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD11	10	0.23
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD12	10	0.23
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD13	10	0.23
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG21	4	0.23
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG22	4	0.23
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG23	4	0.23
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	6	0.23
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	6	0.23
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	6	0.23
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	8	0.23
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	8	0.23
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	8	0.23
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD21	8	0.23
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD22	8	0.23
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD23	8	0.23
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD21	7	0.23
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD22	7	0.23
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD23	7	0.23
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	7	0.23
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	7	0.23
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	7	0.23
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	10	0.23
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	10	0.23
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	10	0.23
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB1	6	0.23
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB2	6	0.23
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB3	6	0.23
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	4	0.23
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	4	0.23
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	4	0.23
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	8	0.23
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	8	0.23
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	8	0.23
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB1	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB2	10	0.23
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB3	10	0.23
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD21	5	0.23
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD22	5	0.23
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD23	5	0.23
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD21	6	0.23
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD22	6	0.23
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD23	6	0.23
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	2	0.23
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	2	0.23
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	2	0.23
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	8	0.23
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	8	0.23
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	8	0.23
(1,793)	1:81:A:ILE:H	1:90:A:THR:HG21	4	0.23
(1,793)	1:81:A:ILE:H	1:90:A:THR:HG22	4	0.23
(1,793)	1:81:A:ILE:H	1:90:A:THR:HG23	4	0.23
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD11	7	0.23
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD12	7	0.23
(1,754)	1:62:A:GLU:H	1:96:A:ILE:HD13	7	0.23
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	7	0.23
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	7	0.23
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	7	0.23
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	9	0.23
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	9	0.23
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	9	0.23
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	4	0.23
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	4	0.23
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	4	0.23
(1,677)	1:20:A:PHE:H	1:171:A:THR:HG21	6	0.23
(1,677)	1:20:A:PHE:H	1:171:A:THR:HG22	6	0.23
(1,677)	1:20:A:PHE:H	1:171:A:THR:HG23	6	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	2	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	2	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	2	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	8	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	8	0.23
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	8	0.23
(1,660)	1:203:A:ILE:H	1:203:A:ILE:HD11	8	0.23
(1,660)	1:203:A:ILE:H	1:203:A:ILE:HD12	8	0.23
(1,660)	1:203:A:ILE:H	1:203:A:ILE:HD13	8	0.23
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD11	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD12	1	0.23
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD13	1	0.23
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD11	4	0.23
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD12	4	0.23
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD13	4	0.23
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	2	0.23
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	2	0.23
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	2	0.23
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	2	0.23
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	2	0.23
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	2	0.23
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	2	0.23
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	2	0.23
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	2	0.23
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	7	0.23
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	7	0.23
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	7	0.23
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	7	0.23
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	7	0.23
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	7	0.23
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	7	0.23
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	7	0.23
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	7	0.23
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	1	0.23
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	1	0.23
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	1	0.23
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	1	0.23
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	1	0.23
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	1	0.23
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	1	0.23
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	1	0.23
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	1	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	8	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	8	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	8	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	8	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	8	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	8	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	8	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	8	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	8	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	10	0.23
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	10	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	10	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	10	0.23
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	10	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	10	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	10	0.23
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	10	0.23
(1,521)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	7	0.23
(1,521)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	7	0.23
(1,521)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	7	0.23
(1,521)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	7	0.23
(1,521)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	7	0.23
(1,521)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	7	0.23
(1,521)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	7	0.23
(1,521)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	7	0.23
(1,521)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	7	0.23
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG21	4	0.23
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG22	4	0.23
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG23	4	0.23
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG21	4	0.23
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG22	4	0.23
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG23	4	0.23
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG21	4	0.23
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG22	4	0.23
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG23	4	0.23
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	8	0.23
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	8	0.23
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	8	0.23
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	8	0.23
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	8	0.23
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	8	0.23
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	8	0.23
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	8	0.23
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	8	0.23
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	10	0.23
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	10	0.23
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	10	0.23
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	10	0.23
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	10	0.23
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	10	0.23
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	10	0.23
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	10	0.23
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	8	0.23
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	8	0.23
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	8	0.23
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	8	0.23
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	8	0.23
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	8	0.23
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	8	0.23
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	8	0.23
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	8	0.23
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	7	0.23
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	7	0.23
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	7	0.23
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	7	0.23
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	7	0.23
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	7	0.23
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	7	0.23
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	7	0.23
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	7	0.23
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	2	0.23
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	2	0.23
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	2	0.23
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	2	0.23
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	2	0.23
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	2	0.23
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	2	0.23
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	2	0.23
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	2	0.23
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	3	0.23
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	3	0.23
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	3	0.23
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	3	0.23
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	3	0.23
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	3	0.23
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	3	0.23
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	3	0.23
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	3	0.23
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	10	0.23
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	10	0.23
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	10	0.23
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	10	0.23
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	10	0.23
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	10	0.23
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	10	0.23
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	10	0.23
(1,342)	1:146:A:GLU:H	1:191:A:LYS:H	9	0.23
(1,87)	1:137:A:GLY:H	1:138:A:PHE:H	9	0.23
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD21	8	0.22
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD22	8	0.22
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD23	8	0.22
(1,1076)	1:211:A:SER:H	1:207:A:VAL:HG21	6	0.22
(1,1076)	1:211:A:SER:H	1:207:A:VAL:HG22	6	0.22
(1,1076)	1:211:A:SER:H	1:207:A:VAL:HG23	6	0.22
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD11	2	0.22
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD12	2	0.22
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD13	2	0.22
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD21	10	0.22
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD22	10	0.22
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD23	10	0.22
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD21	3	0.22
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD22	3	0.22
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD23	3	0.22
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	8	0.22
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	8	0.22
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	8	0.22
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	5	0.22
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	5	0.22
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	5	0.22
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	6	0.22
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	6	0.22
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	6	0.22
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	8	0.22
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	8	0.22
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	8	0.22
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD11	4	0.22
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD12	4	0.22
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD13	4	0.22
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE1	2	0.22
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE2	2	0.22
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE3	2	0.22
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB1	4	0.22
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB2	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB3	4	0.22
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB1	4	0.22
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB2	4	0.22
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB3	4	0.22
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	10	0.22
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	10	0.22
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	10	0.22
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	3	0.22
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	3	0.22
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	3	0.22
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	6	0.22
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	6	0.22
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	6	0.22
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	8	0.22
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	8	0.22
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	8	0.22
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	1	0.22
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	1	0.22
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	1	0.22
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	9	0.22
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	9	0.22
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	9	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	5	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	5	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	5	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	8	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	8	0.22
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	8	0.22
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	1	0.22
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	1	0.22
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	1	0.22
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	10	0.22
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	10	0.22
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	10	0.22
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	10	0.22
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	10	0.22
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	10	0.22
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	10	0.22
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	10	0.22
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	10	0.22
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD11	1	0.22
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD12	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD13	1	0.22
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD11	1	0.22
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD12	1	0.22
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD13	1	0.22
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD11	1	0.22
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD12	1	0.22
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD13	1	0.22
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	3	0.22
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	3	0.22
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	3	0.22
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	3	0.22
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	3	0.22
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	3	0.22
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	3	0.22
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	3	0.22
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	3	0.22
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	3	0.22
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	3	0.22
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	3	0.22
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	3	0.22
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	3	0.22
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	3	0.22
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	3	0.22
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	3	0.22
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	3	0.22
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	2	0.22
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	2	0.22
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	2	0.22
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	2	0.22
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	2	0.22
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	2	0.22
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	2	0.22
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	2	0.22
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	2	0.22
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	5	0.22
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	5	0.22
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	5	0.22
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	5	0.22
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	5	0.22
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	5	0.22
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	5	0.22
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	5	0.22
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE1	1	0.22
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE2	1	0.22
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE3	1	0.22
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE1	1	0.22
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE2	1	0.22
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE3	1	0.22
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE1	1	0.22
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE2	1	0.22
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE3	1	0.22
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	1	0.22
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	1	0.22
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	1	0.22
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	1	0.22
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	1	0.22
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	1	0.22
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	1	0.22
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	1	0.22
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	1	0.22
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	5	0.22
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	5	0.22
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	5	0.22
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	5	0.22
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	5	0.22
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	5	0.22
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	5	0.22
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	5	0.22
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	5	0.22
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	2	0.22
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	2	0.22
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	2	0.22
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	2	0.22
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	2	0.22
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	2	0.22
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	2	0.22
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	2	0.22
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	2	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	1	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	1	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	1	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	1	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	1	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	1	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	1	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	1	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	4	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	4	0.22
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	4	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	4	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	4	0.22
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	4	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	4	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	4	0.22
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	4	0.22
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	8	0.22
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	8	0.22
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	8	0.22
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	8	0.22
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	8	0.22
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	8	0.22
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	8	0.22
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	8	0.22
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	8	0.22
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	1	0.22
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	1	0.22
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	1	0.22
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	1	0.22
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	1	0.22
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	1	0.22
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	1	0.22
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	1	0.22
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	1	0.22
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	6	0.22
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	6	0.22
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	6	0.22
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	6	0.22
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	6	0.22
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	6	0.22
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	6	0.22
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	6	0.22
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	6	0.22
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD11	3	0.22
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD12	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD13	3	0.22
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD11	3	0.22
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD12	3	0.22
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD13	3	0.22
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD11	3	0.22
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD12	3	0.22
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD13	3	0.22
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	10	0.22
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	10	0.22
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	10	0.22
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	10	0.22
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	10	0.22
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	10	0.22
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	10	0.22
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	10	0.22
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	10	0.22
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	5	0.22
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	5	0.22
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	5	0.22
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	5	0.22
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	5	0.22
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	5	0.22
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	5	0.22
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	5	0.22
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	5	0.22
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	3	0.22
(1,282)	1:139:A:TYR:H	1:142:A:TYR:H	4	0.22
(1,69)	1:105:A:ASN:H	1:106:A:ASN:H	9	0.22
(2,142)	1:207:A:VAL:H	1:203:A:ILE:O	4	0.21
(2,80)	1:190:A:LEU:H	1:87:A:ARG:O	7	0.21
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD21	3	0.21
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD22	3	0.21
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD23	3	0.21
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD11	7	0.21
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD12	7	0.21
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD13	7	0.21
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG11	5	0.21
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG12	5	0.21
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG13	5	0.21
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD11	7	0.21
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD12	7	0.21
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD13	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG21	1	0.21
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG22	1	0.21
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG23	1	0.21
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG21	7	0.21
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG22	7	0.21
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG23	7	0.21
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD21	4	0.21
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD22	4	0.21
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD23	4	0.21
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	3	0.21
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	3	0.21
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	3	0.21
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	9	0.21
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	9	0.21
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	9	0.21
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	8	0.21
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	8	0.21
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	8	0.21
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG21	5	0.21
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG22	5	0.21
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG23	5	0.21
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG11	2	0.21
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG12	2	0.21
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG13	2	0.21
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE1	4	0.21
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE2	4	0.21
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE3	4	0.21
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD11	3	0.21
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD12	3	0.21
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD13	3	0.21
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB1	6	0.21
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB2	6	0.21
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB3	6	0.21
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD21	1	0.21
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD22	1	0.21
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD23	1	0.21
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD21	10	0.21
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD22	10	0.21
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD23	10	0.21
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	7	0.21
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	7	0.21
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	3	0.21
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	3	0.21
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	3	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	1	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	1	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	1	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	9	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	9	0.21
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	9	0.21
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD11	3	0.21
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD12	3	0.21
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD13	3	0.21
(1,769)	1:74:A:LYS:H	1:94:A:THR:HG21	7	0.21
(1,769)	1:74:A:LYS:H	1:94:A:THR:HG22	7	0.21
(1,769)	1:74:A:LYS:H	1:94:A:THR:HG23	7	0.21
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	1	0.21
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	1	0.21
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	1	0.21
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB1	1	0.21
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB2	1	0.21
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB3	1	0.21
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB1	1	0.21
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB2	1	0.21
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB3	1	0.21
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG21	8	0.21
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG22	8	0.21
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG23	8	0.21
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG11	4	0.21
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG12	4	0.21
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG13	4	0.21
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG11	7	0.21
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG12	7	0.21
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG13	7	0.21
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD11	10	0.21
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD12	10	0.21
(1,604)	1:33:A:ILE:H	1:33:A:ILE:HD13	10	0.21
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	1	0.21
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	1	0.21
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	1	0.21
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	1	0.21
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	1	0.21
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	1	0.21
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	1	0.21
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	1	0.21
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE1	6	0.21
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE2	6	0.21
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE3	6	0.21
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE1	6	0.21
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE2	6	0.21
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE3	6	0.21
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE1	6	0.21
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE2	6	0.21
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE3	6	0.21
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG21	1	0.21
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG22	1	0.21
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG23	1	0.21
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG21	1	0.21
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG22	1	0.21
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG23	1	0.21
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG21	1	0.21
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG22	1	0.21
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG23	1	0.21
(1,520)	1:103:A:LEU:HD11	1:150:A:VAL:HG11	10	0.21
(1,520)	1:103:A:LEU:HD11	1:150:A:VAL:HG12	10	0.21
(1,520)	1:103:A:LEU:HD11	1:150:A:VAL:HG13	10	0.21
(1,520)	1:103:A:LEU:HD12	1:150:A:VAL:HG11	10	0.21
(1,520)	1:103:A:LEU:HD12	1:150:A:VAL:HG12	10	0.21
(1,520)	1:103:A:LEU:HD12	1:150:A:VAL:HG13	10	0.21
(1,520)	1:103:A:LEU:HD13	1:150:A:VAL:HG11	10	0.21
(1,520)	1:103:A:LEU:HD13	1:150:A:VAL:HG12	10	0.21
(1,520)	1:103:A:LEU:HD13	1:150:A:VAL:HG13	10	0.21
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG11	3	0.21
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG12	3	0.21
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG13	3	0.21
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG11	3	0.21
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG12	3	0.21
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG13	3	0.21
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG11	3	0.21
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG12	3	0.21
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG13	3	0.21
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	10	0.21
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	10	0.21
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	10	0.21
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	10	0.21
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	10	0.21
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	10	0.21
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	10	0.21
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	10	0.21
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	2	0.21
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	2	0.21
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	2	0.21
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	2	0.21
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	2	0.21
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	2	0.21
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	2	0.21
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	2	0.21
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	2	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	6	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	6	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	6	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	6	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	6	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	6	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	6	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	6	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	6	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	9	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	9	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	9	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	9	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	9	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	9	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	9	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	9	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	9	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	10	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	10	0.21
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	10	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	10	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	10	0.21
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	10	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	10	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	10	0.21
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	1	0.21
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	1	0.21
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	1	0.21
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	1	0.21
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	1	0.21
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	1	0.21
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	1	0.21
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	1	0.21
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	1	0.21
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	6	0.21
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	6	0.21
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	6	0.21
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	6	0.21
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	6	0.21
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	6	0.21
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	6	0.21
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	6	0.21
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	6	0.21
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	3	0.21
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	3	0.21
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	3	0.21
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	3	0.21
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	3	0.21
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	3	0.21
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	3	0.21
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	3	0.21
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	3	0.21
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	9	0.21
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	9	0.21
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	9	0.21
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	9	0.21
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	9	0.21
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	9	0.21
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	9	0.21
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	9	0.21
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	9	0.21
(1,473)	1:59:A:ILE:HD11	1:70:A:LEU:HD21	10	0.21
(1,473)	1:59:A:ILE:HD11	1:70:A:LEU:HD22	10	0.21
(1,473)	1:59:A:ILE:HD11	1:70:A:LEU:HD23	10	0.21
(1,473)	1:59:A:ILE:HD12	1:70:A:LEU:HD21	10	0.21
(1,473)	1:59:A:ILE:HD12	1:70:A:LEU:HD22	10	0.21
(1,473)	1:59:A:ILE:HD12	1:70:A:LEU:HD23	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:59:A:ILE:HD13	1:70:A:LEU:HD21	10	0.21
(1,473)	1:59:A:ILE:HD13	1:70:A:LEU:HD22	10	0.21
(1,473)	1:59:A:ILE:HD13	1:70:A:LEU:HD23	10	0.21
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	2	0.21
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	2	0.21
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	2	0.21
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	2	0.21
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	2	0.21
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	2	0.21
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	2	0.21
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	2	0.21
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	2	0.21
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	6	0.21
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	6	0.21
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	6	0.21
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	6	0.21
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	6	0.21
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	6	0.21
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	6	0.21
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	6	0.21
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	6	0.21
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	3	0.21
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	3	0.21
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	3	0.21
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	3	0.21
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	3	0.21
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	3	0.21
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	3	0.21
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	3	0.21
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	3	0.21
(1,422)	1:32:A:LEU:HD21	1:119:A:MET:HE1	3	0.21
(1,422)	1:32:A:LEU:HD21	1:119:A:MET:HE2	3	0.21
(1,422)	1:32:A:LEU:HD21	1:119:A:MET:HE3	3	0.21
(1,422)	1:32:A:LEU:HD22	1:119:A:MET:HE1	3	0.21
(1,422)	1:32:A:LEU:HD22	1:119:A:MET:HE2	3	0.21
(1,422)	1:32:A:LEU:HD22	1:119:A:MET:HE3	3	0.21
(1,422)	1:32:A:LEU:HD23	1:119:A:MET:HE1	3	0.21
(1,422)	1:32:A:LEU:HD23	1:119:A:MET:HE2	3	0.21
(1,422)	1:32:A:LEU:HD23	1:119:A:MET:HE3	3	0.21
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD11	5	0.21
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD12	5	0.21
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD13	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD11	5	0.21
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD12	5	0.21
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD13	5	0.21
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD11	5	0.21
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD12	5	0.21
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD13	5	0.21
(1,407)	1:29:A:LEU:HD11	1:131:A:ILE:HD11	2	0.21
(1,407)	1:29:A:LEU:HD11	1:131:A:ILE:HD12	2	0.21
(1,407)	1:29:A:LEU:HD11	1:131:A:ILE:HD13	2	0.21
(1,407)	1:29:A:LEU:HD12	1:131:A:ILE:HD11	2	0.21
(1,407)	1:29:A:LEU:HD12	1:131:A:ILE:HD12	2	0.21
(1,407)	1:29:A:LEU:HD12	1:131:A:ILE:HD13	2	0.21
(1,407)	1:29:A:LEU:HD13	1:131:A:ILE:HD11	2	0.21
(1,407)	1:29:A:LEU:HD13	1:131:A:ILE:HD12	2	0.21
(1,407)	1:29:A:LEU:HD13	1:131:A:ILE:HD13	2	0.21
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	9	0.21
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	9	0.21
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	9	0.21
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	9	0.21
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	9	0.21
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	9	0.21
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	9	0.21
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	9	0.21
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	9	0.21
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG21	7	0.21
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG22	7	0.21
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG23	7	0.21
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG21	7	0.21
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG22	7	0.21
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG23	7	0.21
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG21	7	0.21
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG22	7	0.21
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG23	7	0.21
(1,336)	1:93:A:ASP:H	1:186:A:VAL:H	7	0.21
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	6	0.21
(1,287)	1:194:A:GLN:H	1:197:A:TYR:H	5	0.21
(1,263)	1:69:A:LYS:H	1:72:A:SER:H	6	0.21
(1,221)	1:180:A:MET:H	1:182:A:ARG:H	1	0.21
(1,167)	1:41:A:LYS:H	1:43:A:ILE:H	10	0.21
(1,134)	1:198:A:LEU:H	1:199:A:GLU:H	5	0.21
(2,98)	1:44:A:PHE:H	1:41:A:LYS:O	10	0.2
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD11	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD12	9	0.2
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD13	9	0.2
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG11	9	0.2
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG12	9	0.2
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG13	9	0.2
(1,1039)	1:198:A:LEU:H	1:195:A:THR:HG21	3	0.2
(1,1039)	1:198:A:LEU:H	1:195:A:THR:HG22	3	0.2
(1,1039)	1:198:A:LEU:H	1:195:A:THR:HG23	3	0.2
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG21	4	0.2
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG22	4	0.2
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG23	4	0.2
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD21	2	0.2
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD22	2	0.2
(1,1017)	1:189:A:HIS:H	1:188:A:LEU:HD23	2	0.2
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	6	0.2
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	6	0.2
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	6	0.2
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG11	8	0.2
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG12	8	0.2
(1,960)	1:163:A:GLU:H	1:172:A:VAL:HG13	8	0.2
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	5	0.2
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	5	0.2
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	5	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG21	5	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG22	5	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG23	5	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG21	10	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG22	10	0.2
(1,947)	1:161:A:ALA:H	1:172:A:VAL:HG23	10	0.2
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG21	7	0.2
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG22	7	0.2
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG23	7	0.2
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG21	3	0.2
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG22	3	0.2
(1,937)	1:151:A:ILE:H	1:186:A:VAL:HG23	3	0.2
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	2	0.2
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	2	0.2
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	2	0.2
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB1	9	0.2
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB2	9	0.2
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB3	9	0.2
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	3	0.2
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	3	0.2
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	10	0.2
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	10	0.2
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	10	0.2
(1,739)	1:58:A:LYS:H	1:96:A:ILE:HD11	3	0.2
(1,739)	1:58:A:LYS:H	1:96:A:ILE:HD12	3	0.2
(1,739)	1:58:A:LYS:H	1:96:A:ILE:HD13	3	0.2
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	5	0.2
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	5	0.2
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	5	0.2
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	10	0.2
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	10	0.2
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	10	0.2
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	6	0.2
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	6	0.2
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	6	0.2
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	4	0.2
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	4	0.2
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	4	0.2
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB1	5	0.2
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB2	5	0.2
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB3	5	0.2
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG21	6	0.2
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG22	6	0.2
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG23	6	0.2
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	8	0.2
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	8	0.2
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	8	0.2
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	8	0.2
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	8	0.2
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	8	0.2
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	8	0.2
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	8	0.2
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	8	0.2
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	1	0.2
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	1	0.2
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	1	0.2
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	1	0.2
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	1	0.2
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	1	0.2
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	1	0.2
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	1	0.2
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG21	5	0.2
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG22	5	0.2
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG23	5	0.2
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG21	5	0.2
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG22	5	0.2
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG23	5	0.2
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG21	5	0.2
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG22	5	0.2
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG23	5	0.2
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	2	0.2
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	2	0.2
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	2	0.2
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	2	0.2
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	2	0.2
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	2	0.2
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	2	0.2
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	2	0.2
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	2	0.2
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	3	0.2
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	3	0.2
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	3	0.2
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	3	0.2
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	3	0.2
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	3	0.2
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	3	0.2
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	3	0.2
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	3	0.2
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG11	6	0.2
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG12	6	0.2
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG13	6	0.2
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG11	6	0.2
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG12	6	0.2
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG13	6	0.2
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG11	6	0.2
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG12	6	0.2
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG13	6	0.2
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	7	0.2
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	7	0.2
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	7	0.2
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	7	0.2
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	7	0.2
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	7	0.2
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	7	0.2
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	7	0.2
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	9	0.2
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	9	0.2
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	9	0.2
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	9	0.2
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	9	0.2
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	9	0.2
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	9	0.2
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	9	0.2
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	9	0.2
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	9	0.2
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	9	0.2
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	9	0.2
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	9	0.2
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	9	0.2
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	9	0.2
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	9	0.2
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	9	0.2
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	9	0.2
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	3	0.2
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	3	0.2
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	3	0.2
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	3	0.2
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	3	0.2
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	3	0.2
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	3	0.2
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	3	0.2
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	3	0.2
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	7	0.2
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	7	0.2
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	7	0.2
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	7	0.2
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	7	0.2
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	7	0.2
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	7	0.2
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	7	0.2
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	7	0.2
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	4	0.2
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	4	0.2
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	4	0.2
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	4	0.2
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	4	0.2
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	4	0.2
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	4	0.2
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	4	0.2
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	6	0.2
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	6	0.2
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	6	0.2
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	6	0.2
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	6	0.2
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	6	0.2
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	6	0.2
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	6	0.2
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	6	0.2
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	7	0.2
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	7	0.2
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	7	0.2
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	7	0.2
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	7	0.2
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	7	0.2
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	7	0.2
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	7	0.2
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	7	0.2
(1,280)	1:136:A:VAL:H	1:139:A:TYR:H	5	0.2
(1,167)	1:41:A:LYS:H	1:43:A:ILE:H	5	0.2
(1,131)	1:195:A:THR:H	1:196:A:GLU:H	1	0.2
(1,87)	1:137:A:GLY:H	1:138:A:PHE:H	4	0.2
(2,82)	1:28:A:GLN:H	1:24:A:ALA:O	2	0.19
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	9	0.19
(2,16)	1:79:A:ASN:H	1:92:A:VAL:O	1	0.19
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG21	9	0.19
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG22	9	0.19
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG23	9	0.19
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG21	8	0.19
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG22	8	0.19
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG23	8	0.19
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	1	0.19
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	1	0.19
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD21	5	0.19
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD22	5	0.19
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD23	5	0.19
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD21	5	0.19
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD22	5	0.19
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD23	5	0.19
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	4	0.19
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	4	0.19
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	4	0.19
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	6	0.19
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	6	0.19
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	6	0.19
(1,944)	1:160:A:TYR:H	1:152:A:THR:HG21	3	0.19
(1,944)	1:160:A:TYR:H	1:152:A:THR:HG22	3	0.19
(1,944)	1:160:A:TYR:H	1:152:A:THR:HG23	3	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	3	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	3	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	3	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	10	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	10	0.19
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	10	0.19
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD11	2	0.19
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD12	2	0.19
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD13	2	0.19
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE1	6	0.19
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE2	6	0.19
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE3	6	0.19
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB1	6	0.19
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB2	6	0.19
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB3	6	0.19
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB1	4	0.19
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB2	4	0.19
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB3	4	0.19
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB1	5	0.19
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB2	5	0.19
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB3	5	0.19
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	2	0.19
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	2	0.19
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	2	0.19
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD11	10	0.19
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD12	10	0.19
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD13	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	8	0.19
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	8	0.19
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	8	0.19
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	2	0.19
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	2	0.19
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	2	0.19
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD21	10	0.19
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD22	10	0.19
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD23	10	0.19
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	10	0.19
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	10	0.19
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	10	0.19
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD11	10	0.19
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD12	10	0.19
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD13	10	0.19
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	7	0.19
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	7	0.19
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	7	0.19
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	8	0.19
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	8	0.19
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	8	0.19
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB1	5	0.19
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB2	5	0.19
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB3	5	0.19
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	9	0.19
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	9	0.19
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	9	0.19
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB1	6	0.19
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB2	6	0.19
(1,687)	1:27:A:ALA:H	1:111:A:ALA:HB3	6	0.19
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG11	4	0.19
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG12	4	0.19
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG13	4	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	1	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	1	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	1	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	5	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	5	0.19
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	5	0.19
(1,650)	1:172:A:VAL:H	1:172:A:VAL:HG21	4	0.19
(1,650)	1:172:A:VAL:H	1:172:A:VAL:HG22	4	0.19
(1,650)	1:172:A:VAL:H	1:172:A:VAL:HG23	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	3	0.19
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	3	0.19
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	3	0.19
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	3	0.19
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	3	0.19
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	3	0.19
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	3	0.19
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	3	0.19
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	3	0.19
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	4	0.19
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	4	0.19
(1,590)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	4	0.19
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	4	0.19
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	4	0.19
(1,590)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	4	0.19
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	4	0.19
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	4	0.19
(1,590)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	4	0.19
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG21	8	0.19
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG22	8	0.19
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG23	8	0.19
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG21	8	0.19
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG22	8	0.19
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG23	8	0.19
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG21	8	0.19
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG22	8	0.19
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG23	8	0.19
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	9	0.19
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	9	0.19
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	9	0.19
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	9	0.19
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	9	0.19
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	9	0.19
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	9	0.19
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	9	0.19
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	9	0.19
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG21	10	0.19
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG22	10	0.19
(1,570)	1:150:A:VAL:HG21	1:184:A:THR:HG23	10	0.19
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG21	10	0.19
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG22	10	0.19
(1,570)	1:150:A:VAL:HG22	1:184:A:THR:HG23	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG21	10	0.19
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG22	10	0.19
(1,570)	1:150:A:VAL:HG23	1:184:A:THR:HG23	10	0.19
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE1	3	0.19
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE2	3	0.19
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE3	3	0.19
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE1	3	0.19
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE2	3	0.19
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE3	3	0.19
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE1	3	0.19
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE2	3	0.19
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE3	3	0.19
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	2	0.19
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	2	0.19
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	2	0.19
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	2	0.19
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	2	0.19
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	2	0.19
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	2	0.19
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	2	0.19
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	2	0.19
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	6	0.19
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	6	0.19
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	6	0.19
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	6	0.19
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	6	0.19
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	6	0.19
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	6	0.19
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	6	0.19
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	6	0.19
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB1	7	0.19
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB2	7	0.19
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB3	7	0.19
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB1	7	0.19
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB2	7	0.19
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB3	7	0.19
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB1	7	0.19
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB2	7	0.19
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB3	7	0.19
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE1	8	0.19
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE2	8	0.19
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE3	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE1	8	0.19
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE2	8	0.19
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE3	8	0.19
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE1	8	0.19
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE2	8	0.19
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE3	8	0.19
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE1	9	0.19
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE2	9	0.19
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE3	9	0.19
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE1	9	0.19
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE2	9	0.19
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE3	9	0.19
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE1	9	0.19
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE2	9	0.19
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE3	9	0.19
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	8	0.19
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	8	0.19
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	8	0.19
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	8	0.19
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	8	0.19
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	8	0.19
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	8	0.19
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	8	0.19
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	8	0.19
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	1	0.19
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	1	0.19
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	1	0.19
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	1	0.19
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	1	0.19
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	1	0.19
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	1	0.19
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	1	0.19
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	1	0.19
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	8	0.19
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	8	0.19
(1,485)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	8	0.19
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	8	0.19
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	8	0.19
(1,485)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	8	0.19
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	8	0.19
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	8	0.19
(1,485)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	7	0.19
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	7	0.19
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	7	0.19
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	7	0.19
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	7	0.19
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	7	0.19
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	7	0.19
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	7	0.19
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	7	0.19
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	1	0.19
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	1	0.19
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	1	0.19
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	1	0.19
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	1	0.19
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	1	0.19
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	1	0.19
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	1	0.19
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	1	0.19
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD21	5	0.19
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD22	5	0.19
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD23	5	0.19
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD21	5	0.19
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD22	5	0.19
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD23	5	0.19
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD21	5	0.19
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD22	5	0.19
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD23	5	0.19
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	3	0.19
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	3	0.19
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	3	0.19
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	3	0.19
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	3	0.19
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	3	0.19
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	3	0.19
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	3	0.19
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	3	0.19
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	5	0.19
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	5	0.19
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	5	0.19
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	5	0.19
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	5	0.19
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	5	0.19
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	5	0.19
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	5	0.19
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	3	0.19
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	3	0.19
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	3	0.19
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	3	0.19
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	3	0.19
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	3	0.19
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	3	0.19
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	3	0.19
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	3	0.19
(1,364)	1:225:A:GLU:H	1:230:A:VAL:H	1	0.19
(1,325)	1:80:A:LEU:H	1:221:A:PHE:H	5	0.19
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	8	0.19
(1,289)	1:199:A:GLU:H	1:202:A:ARG:H	1	0.19
(1,247)	1:223:A:GLU:H	1:225:A:GLU:H	8	0.19
(1,193)	1:72:A:SER:H	1:74:A:LYS:H	10	0.19
(1,109)	1:167:A:GLY:H	1:168:A:GLY:H	4	0.19
(1,69)	1:105:A:ASN:H	1:106:A:ASN:H	8	0.19
(1,63)	1:96:A:ILE:H	1:97:A:GLY:H	4	0.19
(1,47)	1:76:A:LEU:H	1:77:A:HIS:H	9	0.19
(1,16)	1:38:A:TYR:H	1:39:A:SER:H	8	0.19
(2,84)	1:29:A:LEU:H	1:25:A:GLU:O	4	0.18
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	6	0.18
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG21	2	0.18
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG22	2	0.18
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG23	2	0.18
(1,1082)	1:216:A:TYR:H	1:78:A:ILE:HD11	4	0.18
(1,1082)	1:216:A:TYR:H	1:78:A:ILE:HD12	4	0.18
(1,1082)	1:216:A:TYR:H	1:78:A:ILE:HD13	4	0.18
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG11	5	0.18
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG12	5	0.18
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG13	5	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG11	1	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG12	1	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG13	1	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG11	6	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG12	6	0.18
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG13	6	0.18
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB1	2	0.18
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB3	2	0.18
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG21	2	0.18
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG22	2	0.18
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG23	2	0.18
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG21	9	0.18
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG22	9	0.18
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG23	9	0.18
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	9	0.18
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	9	0.18
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	9	0.18
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG21	6	0.18
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG22	6	0.18
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG23	6	0.18
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	6	0.18
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	6	0.18
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	6	0.18
(1,900)	1:141:A:ALA:H	1:188:A:LEU:HD21	3	0.18
(1,900)	1:141:A:ALA:H	1:188:A:LEU:HD22	3	0.18
(1,900)	1:141:A:ALA:H	1:188:A:LEU:HD23	3	0.18
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG21	2	0.18
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG22	2	0.18
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG23	2	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	1	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	1	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	1	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	7	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	7	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	7	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	8	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	8	0.18
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	8	0.18
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD21	1	0.18
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD22	1	0.18
(1,838)	1:95:A:GLY:H	1:56:A:LEU:HD23	1	0.18
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	6	0.18
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	6	0.18
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	6	0.18
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	2	0.18
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	2	0.18
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	2	0.18
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	1	0.18
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	1	0.18
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD11	7	0.18
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD12	7	0.18
(1,799)	1:83:A:ASN:H	1:89:A:LEU:HD13	7	0.18
(1,764)	1:70:A:LEU:H	1:59:A:ILE:HD11	9	0.18
(1,764)	1:70:A:LEU:H	1:59:A:ILE:HD12	9	0.18
(1,764)	1:70:A:LEU:H	1:59:A:ILE:HD13	9	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	3	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	3	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	3	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	6	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	6	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	6	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	9	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	9	0.18
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	9	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	3	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	3	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	3	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	8	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	8	0.18
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	8	0.18
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	10	0.18
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	10	0.18
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	10	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	8	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	8	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	8	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	9	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	9	0.18
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	9	0.18
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG21	7	0.18
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG22	7	0.18
(1,680)	1:21:A:ALA:H	1:109:A:THR:HG23	7	0.18
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG11	7	0.18
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG12	7	0.18
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG13	7	0.18
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	3	0.18
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	3	0.18
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	3	0.18
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	10	0.18
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	10	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG11	1	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG12	1	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG13	1	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG11	10	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG12	10	0.18
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG13	10	0.18
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG21	5	0.18
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG22	5	0.18
(1,582)	1:190:A:LEU:HD11	1:195:A:THR:HG23	5	0.18
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG21	5	0.18
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG22	5	0.18
(1,582)	1:190:A:LEU:HD12	1:195:A:THR:HG23	5	0.18
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG21	5	0.18
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG22	5	0.18
(1,582)	1:190:A:LEU:HD13	1:195:A:THR:HG23	5	0.18
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	10	0.18
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	10	0.18
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	10	0.18
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	10	0.18
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	10	0.18
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	10	0.18
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	10	0.18
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	10	0.18
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	10	0.18
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	6	0.18
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	6	0.18
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	6	0.18
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	6	0.18
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	6	0.18
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	6	0.18
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	6	0.18
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	6	0.18
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	6	0.18
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	2	0.18
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	2	0.18
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	2	0.18
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	2	0.18
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	2	0.18
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	2	0.18
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	2	0.18
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	2	0.18
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD21	4	0.18
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD22	4	0.18
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD23	4	0.18
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD21	4	0.18
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD22	4	0.18
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD23	4	0.18
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD21	4	0.18
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD22	4	0.18
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD23	4	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	1	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	1	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	1	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	1	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	1	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	1	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	1	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	1	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	1	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	7	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	7	0.18
(1,503)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	7	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	7	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	7	0.18
(1,503)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	7	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	7	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	7	0.18
(1,503)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	7	0.18
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	6	0.18
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	6	0.18
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	6	0.18
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	6	0.18
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	6	0.18
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	6	0.18
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	6	0.18
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	6	0.18
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	6	0.18
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	2	0.18
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	2	0.18
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	2	0.18
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	2	0.18
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	2	0.18
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	2	0.18
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	2	0.18
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	2	0.18
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	10	0.18
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	10	0.18
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	10	0.18
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	10	0.18
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	10	0.18
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	10	0.18
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	10	0.18
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	10	0.18
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	10	0.18
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	10	0.18
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	10	0.18
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	10	0.18
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	10	0.18
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	10	0.18
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	10	0.18
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	10	0.18
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	10	0.18
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	10	0.18
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	9	0.18
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	9	0.18
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	9	0.18
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	9	0.18
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	9	0.18
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	9	0.18
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	9	0.18
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	9	0.18
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	9	0.18
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	9	0.18
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	9	0.18
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	9	0.18
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	9	0.18
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	9	0.18
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	9	0.18
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	9	0.18
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	9	0.18
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	9	0.18
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	5	0.18
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	5	0.18
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	5	0.18
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	5	0.18
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	5	0.18
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	5	0.18
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	5	0.18
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	5	0.18
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	10	0.18
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	10	0.18
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	10	0.18
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	10	0.18
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	10	0.18
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	10	0.18
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	10	0.18
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	10	0.18
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	10	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	7	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	7	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	7	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	7	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	7	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	7	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	7	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	7	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	7	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	10	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	10	0.18
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	10	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	10	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	10	0.18
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	10	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	10	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	10	0.18
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	10	0.18
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	4	0.18
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	4	0.18
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	4	0.18
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	4	0.18
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	4	0.18
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	4	0.18
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	4	0.18
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	4	0.18
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG21	6	0.18
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG22	6	0.18
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG23	6	0.18
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG21	6	0.18
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG22	6	0.18
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG23	6	0.18
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG21	6	0.18
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG22	6	0.18
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG23	6	0.18
(1,314)	1:58:A:LYS:H	1:96:A:ILE:H	8	0.18
(1,288)	1:196:A:GLU:H	1:199:A:GLU:H	1	0.18
(1,270)	1:104:A:ILE:H	1:107:A:LEU:H	1	0.18
(1,110)	1:168:A:GLY:H	1:169:A:SER:H	6	0.18
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	8	0.17
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD21	5	0.17
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD22	5	0.17
(1,1112)	1:123:A:GLN:HE21	1:122:A:LEU:HD23	5	0.17
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG11	1	0.17
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG12	1	0.17
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG13	1	0.17
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG11	2	0.17
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG12	2	0.17
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG13	2	0.17
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD11	3	0.17
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD12	3	0.17
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD13	3	0.17
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG11	4	0.17
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG12	4	0.17
(1,1074)	1:210:A:HIS:H	1:207:A:VAL:HG13	4	0.17
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG21	10	0.17
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG22	10	0.17
(1,1073)	1:209:A:LYS:H	1:207:A:VAL:HG23	10	0.17
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD11	4	0.17
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD12	4	0.17
(1,1067)	1:207:A:VAL:H	1:80:A:LEU:HD13	4	0.17
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD11	9	0.17
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD12	9	0.17
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD13	9	0.17
(1,1025)	1:191:A:LYS:H	1:190:A:LEU:HD21	3	0.17
(1,1025)	1:191:A:LYS:H	1:190:A:LEU:HD22	3	0.17
(1,1025)	1:191:A:LYS:H	1:190:A:LEU:HD23	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	3	0.17
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	3	0.17
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	3	0.17
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	4	0.17
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	4	0.17
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	4	0.17
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG21	4	0.17
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG22	4	0.17
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG23	4	0.17
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG21	3	0.17
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG22	3	0.17
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG23	3	0.17
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG21	8	0.17
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG22	8	0.17
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG23	8	0.17
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	7	0.17
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	7	0.17
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	7	0.17
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD11	6	0.17
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD12	6	0.17
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD13	6	0.17
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD11	5	0.17
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD12	5	0.17
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD13	5	0.17
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD11	6	0.17
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD12	6	0.17
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD13	6	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB1	1	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB2	1	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB3	1	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB1	5	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB2	5	0.17
(1,871)	1:126:A:ALA:H	1:121:A:ALA:HB3	5	0.17
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB1	8	0.17
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB2	8	0.17
(1,857)	1:118:A:PHE:H	1:121:A:ALA:HB3	8	0.17
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD11	3	0.17
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD12	3	0.17
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD13	3	0.17
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	4	0.17
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	4	0.17
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB1	2	0.17
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB2	2	0.17
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB3	2	0.17
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB1	7	0.17
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB2	7	0.17
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB3	7	0.17
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE1	3	0.17
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE2	3	0.17
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE3	3	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	6	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	6	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	6	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	8	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	8	0.17
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	8	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	1	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	1	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	1	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	8	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	8	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	8	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	9	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	9	0.17
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	9	0.17
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG21	7	0.17
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG22	7	0.17
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG23	7	0.17
(1,770)	1:75:A:GLU:H	1:70:A:LEU:HD11	9	0.17
(1,770)	1:75:A:GLU:H	1:70:A:LEU:HD12	9	0.17
(1,770)	1:75:A:GLU:H	1:70:A:LEU:HD13	9	0.17
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	4	0.17
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	4	0.17
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	4	0.17
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	6	0.17
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	6	0.17
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	6	0.17
(1,734)	1:55:A:ALA:H	1:56:A:LEU:HD21	2	0.17
(1,734)	1:55:A:ALA:H	1:56:A:LEU:HD22	2	0.17
(1,734)	1:55:A:ALA:H	1:56:A:LEU:HD23	2	0.17
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD11	5	0.17
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD12	5	0.17
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD13	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	1	0.17
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	1	0.17
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	1	0.17
(1,693)	1:31:A:SER:H	1:30:A:MET:HE1	3	0.17
(1,693)	1:31:A:SER:H	1:30:A:MET:HE2	3	0.17
(1,693)	1:31:A:SER:H	1:30:A:MET:HE3	3	0.17
(1,692)	1:29:A:LEU:H	1:119:A:MET:HE1	3	0.17
(1,692)	1:29:A:LEU:H	1:119:A:MET:HE2	3	0.17
(1,692)	1:29:A:LEU:H	1:119:A:MET:HE3	3	0.17
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	8	0.17
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	8	0.17
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	8	0.17
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	5	0.17
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	5	0.17
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	5	0.17
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	10	0.17
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	10	0.17
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	10	0.17
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG11	2	0.17
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG12	2	0.17
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG13	2	0.17
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD11	8	0.17
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD12	8	0.17
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD13	8	0.17
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD11	9	0.17
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD12	9	0.17
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD13	9	0.17
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	7	0.17
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	7	0.17
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	7	0.17
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	7	0.17
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	7	0.17
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	7	0.17
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	7	0.17
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	7	0.17
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	7	0.17
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	8	0.17
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	8	0.17
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	8	0.17
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	8	0.17
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	8	0.17
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	8	0.17
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	8	0.17
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	8	0.17
(1,575)	1:174:A:THR:HG21	1:176:A:THR:HG21	2	0.17
(1,575)	1:174:A:THR:HG21	1:176:A:THR:HG22	2	0.17
(1,575)	1:174:A:THR:HG21	1:176:A:THR:HG23	2	0.17
(1,575)	1:174:A:THR:HG22	1:176:A:THR:HG21	2	0.17
(1,575)	1:174:A:THR:HG22	1:176:A:THR:HG22	2	0.17
(1,575)	1:174:A:THR:HG22	1:176:A:THR:HG23	2	0.17
(1,575)	1:174:A:THR:HG23	1:176:A:THR:HG21	2	0.17
(1,575)	1:174:A:THR:HG23	1:176:A:THR:HG22	2	0.17
(1,575)	1:174:A:THR:HG23	1:176:A:THR:HG23	2	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	4	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	4	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	4	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	4	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	4	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	4	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	4	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	4	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	4	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	5	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	5	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	5	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	5	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	5	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	5	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	5	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	5	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	5	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	6	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	6	0.17
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	6	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	6	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	6	0.17
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	6	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	6	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	6	0.17
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	6	0.17
(1,555)	1:144:A:VAL:HG11	1:188:A:LEU:HD21	1	0.17
(1,555)	1:144:A:VAL:HG11	1:188:A:LEU:HD22	1	0.17
(1,555)	1:144:A:VAL:HG11	1:188:A:LEU:HD23	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:144:A:VAL:HG12	1:188:A:LEU:HD21	1	0.17
(1,555)	1:144:A:VAL:HG12	1:188:A:LEU:HD22	1	0.17
(1,555)	1:144:A:VAL:HG12	1:188:A:LEU:HD23	1	0.17
(1,555)	1:144:A:VAL:HG13	1:188:A:LEU:HD21	1	0.17
(1,555)	1:144:A:VAL:HG13	1:188:A:LEU:HD22	1	0.17
(1,555)	1:144:A:VAL:HG13	1:188:A:LEU:HD23	1	0.17
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	4	0.17
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	4	0.17
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	4	0.17
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	4	0.17
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	4	0.17
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	4	0.17
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	4	0.17
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	4	0.17
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	4	0.17
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	2	0.17
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	2	0.17
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	2	0.17
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	2	0.17
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	2	0.17
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	2	0.17
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	2	0.17
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	2	0.17
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	2	0.17
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	9	0.17
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	9	0.17
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	9	0.17
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	9	0.17
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	9	0.17
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	9	0.17
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	9	0.17
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	9	0.17
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	9	0.17
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	6	0.17
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	6	0.17
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	6	0.17
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	6	0.17
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	6	0.17
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	6	0.17
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	6	0.17
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	6	0.17
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	4	0.17
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	4	0.17
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	4	0.17
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	4	0.17
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	4	0.17
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	4	0.17
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	4	0.17
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	4	0.17
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	4	0.17
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	6	0.17
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	6	0.17
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	6	0.17
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	6	0.17
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	6	0.17
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	6	0.17
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	6	0.17
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	6	0.17
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	6	0.17
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	1	0.17
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	1	0.17
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	1	0.17
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	1	0.17
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	1	0.17
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	1	0.17
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	1	0.17
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	1	0.17
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	1	0.17
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	5	0.17
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	5	0.17
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	5	0.17
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	5	0.17
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	5	0.17
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	5	0.17
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	5	0.17
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	5	0.17
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	5	0.17
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	9	0.17
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	9	0.17
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	9	0.17
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	9	0.17
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	9	0.17
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	9	0.17
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	9	0.17
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	9	0.17
(1,478)	1:78:A:ILE:HD11	1:214:A:ILE:HD11	6	0.17
(1,478)	1:78:A:ILE:HD11	1:214:A:ILE:HD12	6	0.17
(1,478)	1:78:A:ILE:HD11	1:214:A:ILE:HD13	6	0.17
(1,478)	1:78:A:ILE:HD12	1:214:A:ILE:HD11	6	0.17
(1,478)	1:78:A:ILE:HD12	1:214:A:ILE:HD12	6	0.17
(1,478)	1:78:A:ILE:HD12	1:214:A:ILE:HD13	6	0.17
(1,478)	1:78:A:ILE:HD13	1:214:A:ILE:HD11	6	0.17
(1,478)	1:78:A:ILE:HD13	1:214:A:ILE:HD12	6	0.17
(1,478)	1:78:A:ILE:HD13	1:214:A:ILE:HD13	6	0.17
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	7	0.17
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	7	0.17
(1,468)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	7	0.17
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	7	0.17
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	7	0.17
(1,468)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	7	0.17
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	7	0.17
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	7	0.17
(1,468)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	7	0.17
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	5	0.17
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	5	0.17
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	5	0.17
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	5	0.17
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	5	0.17
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	5	0.17
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	5	0.17
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	5	0.17
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	5	0.17
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	9	0.17
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	9	0.17
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	9	0.17
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	9	0.17
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	9	0.17
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	9	0.17
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	9	0.17
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	9	0.17
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	9	0.17
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD21	8	0.17
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD22	8	0.17
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD23	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD21	8	0.17
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD22	8	0.17
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD23	8	0.17
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD21	8	0.17
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD22	8	0.17
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD23	8	0.17
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	7	0.17
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	7	0.17
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	7	0.17
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	7	0.17
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	7	0.17
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	7	0.17
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	7	0.17
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	7	0.17
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	7	0.17
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	4	0.17
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	4	0.17
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	4	0.17
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	4	0.17
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	4	0.17
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	4	0.17
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	4	0.17
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	4	0.17
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	4	0.17
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG11	4	0.17
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG12	4	0.17
(1,408)	1:29:A:LEU:HD11	1:136:A:VAL:HG13	4	0.17
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG11	4	0.17
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG12	4	0.17
(1,408)	1:29:A:LEU:HD12	1:136:A:VAL:HG13	4	0.17
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG11	4	0.17
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG12	4	0.17
(1,408)	1:29:A:LEU:HD13	1:136:A:VAL:HG13	4	0.17
(1,406)	1:29:A:LEU:HD11	1:122:A:LEU:HD21	8	0.17
(1,406)	1:29:A:LEU:HD11	1:122:A:LEU:HD22	8	0.17
(1,406)	1:29:A:LEU:HD11	1:122:A:LEU:HD23	8	0.17
(1,406)	1:29:A:LEU:HD12	1:122:A:LEU:HD21	8	0.17
(1,406)	1:29:A:LEU:HD12	1:122:A:LEU:HD22	8	0.17
(1,406)	1:29:A:LEU:HD12	1:122:A:LEU:HD23	8	0.17
(1,406)	1:29:A:LEU:HD13	1:122:A:LEU:HD21	8	0.17
(1,406)	1:29:A:LEU:HD13	1:122:A:LEU:HD22	8	0.17
(1,406)	1:29:A:LEU:HD13	1:122:A:LEU:HD23	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:131:A:ILE:H	1:134:A:PHE:H	8	0.17
(1,263)	1:69:A:LYS:H	1:72:A:SER:H	3	0.17
(1,194)	1:81:A:ILE:H	1:83:A:ASN:H	2	0.17
(1,167)	1:41:A:LYS:H	1:43:A:ILE:H	8	0.17
(1,61)	1:94:A:THR:H	1:95:A:GLY:H	7	0.17
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	3	0.16
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	9	0.16
(2,28)	1:83:A:ASN:H	1:88:A:THR:O	2	0.16
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG21	10	0.16
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG22	10	0.16
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG23	10	0.16
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG11	8	0.16
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG12	8	0.16
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG13	8	0.16
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD11	1	0.16
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD12	1	0.16
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD13	1	0.16
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG11	10	0.16
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG12	10	0.16
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG13	10	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG21	2	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG22	2	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG23	2	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG21	8	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG22	8	0.16
(1,1023)	1:191:A:LYS:H	1:144:A:VAL:HG23	8	0.16
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	9	0.16
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	9	0.16
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	9	0.16
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	8	0.16
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	8	0.16
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	8	0.16
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG21	9	0.16
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG22	9	0.16
(1,968)	1:172:A:VAL:H	1:171:A:THR:HG23	9	0.16
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG21	7	0.16
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG22	7	0.16
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG23	7	0.16
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB1	3	0.16
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB2	3	0.16
(1,964)	1:169:A:SER:H	1:166:A:ALA:HB3	3	0.16
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG21	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG22	6	0.16
(1,952)	1:162:A:TRP:H	1:150:A:VAL:HG23	6	0.16
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	5	0.16
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	5	0.16
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	5	0.16
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG21	5	0.16
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG22	5	0.16
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG23	5	0.16
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD11	3	0.16
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD12	3	0.16
(1,881)	1:131:A:ILE:H	1:43:A:ILE:HD13	3	0.16
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD11	1	0.16
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD12	1	0.16
(1,851)	1:107:A:LEU:H	1:103:A:LEU:HD13	1	0.16
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	5	0.16
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	5	0.16
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	5	0.16
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG21	5	0.16
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG22	5	0.16
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG23	5	0.16
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	5	0.16
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	5	0.16
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	5	0.16
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD11	10	0.16
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD12	10	0.16
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD13	10	0.16
(1,747)	1:60:A:ARG:H	1:96:A:ILE:HD11	4	0.16
(1,747)	1:60:A:ARG:H	1:96:A:ILE:HD12	4	0.16
(1,747)	1:60:A:ARG:H	1:96:A:ILE:HD13	4	0.16
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	4	0.16
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	4	0.16
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	4	0.16
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	4	0.16
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	4	0.16
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	4	0.16
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	6	0.16
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	6	0.16
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	6	0.16
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB1	8	0.16
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB2	8	0.16
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB3	8	0.16
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG11	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG12	1	0.16
(1,678)	1:20:A:PHE:H	1:172:A:VAL:HG13	1	0.16
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	5	0.16
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	5	0.16
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	5	0.16
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	6	0.16
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	6	0.16
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	6	0.16
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	4	0.16
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	4	0.16
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	4	0.16
(1,634)	1:122:A:LEU:H	1:122:A:LEU:HD11	1	0.16
(1,634)	1:122:A:LEU:H	1:122:A:LEU:HD12	1	0.16
(1,634)	1:122:A:LEU:H	1:122:A:LEU:HD13	1	0.16
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG11	9	0.16
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG12	9	0.16
(1,593)	1:220:A:LEU:HD11	1:222:A:VAL:HG13	9	0.16
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG11	9	0.16
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG12	9	0.16
(1,593)	1:220:A:LEU:HD12	1:222:A:VAL:HG13	9	0.16
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG11	9	0.16
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG12	9	0.16
(1,593)	1:220:A:LEU:HD13	1:222:A:VAL:HG13	9	0.16
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD11	2	0.16
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD12	2	0.16
(1,592)	1:214:A:ILE:HD11	1:218:A:ILE:HD13	2	0.16
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD11	2	0.16
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD12	2	0.16
(1,592)	1:214:A:ILE:HD12	1:218:A:ILE:HD13	2	0.16
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD11	2	0.16
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD12	2	0.16
(1,592)	1:214:A:ILE:HD13	1:218:A:ILE:HD13	2	0.16
(1,584)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	3	0.16
(1,584)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	3	0.16
(1,584)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	3	0.16
(1,584)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	3	0.16
(1,584)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	3	0.16
(1,584)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	3	0.16
(1,584)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	3	0.16
(1,584)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	3	0.16
(1,584)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	3	0.16
(1,557)	1:144:A:VAL:HG21	1:188:A:LEU:HD11	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:144:A:VAL:HG21	1:188:A:LEU:HD12	1	0.16
(1,557)	1:144:A:VAL:HG21	1:188:A:LEU:HD13	1	0.16
(1,557)	1:144:A:VAL:HG22	1:188:A:LEU:HD11	1	0.16
(1,557)	1:144:A:VAL:HG22	1:188:A:LEU:HD12	1	0.16
(1,557)	1:144:A:VAL:HG22	1:188:A:LEU:HD13	1	0.16
(1,557)	1:144:A:VAL:HG23	1:188:A:LEU:HD11	1	0.16
(1,557)	1:144:A:VAL:HG23	1:188:A:LEU:HD12	1	0.16
(1,557)	1:144:A:VAL:HG23	1:188:A:LEU:HD13	1	0.16
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	2	0.16
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	2	0.16
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	2	0.16
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	2	0.16
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	2	0.16
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	2	0.16
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	2	0.16
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	2	0.16
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	2	0.16
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE1	1	0.16
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE2	1	0.16
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE3	1	0.16
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE1	1	0.16
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE2	1	0.16
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE3	1	0.16
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE1	1	0.16
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE2	1	0.16
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE3	1	0.16
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	1	0.16
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	1	0.16
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	1	0.16
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	1	0.16
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	1	0.16
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	1	0.16
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	1	0.16
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	1	0.16
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	1	0.16
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG11	5	0.16
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG12	5	0.16
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG13	5	0.16
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG11	5	0.16
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG12	5	0.16
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG13	5	0.16
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG11	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG12	5	0.16
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG13	5	0.16
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE1	1	0.16
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE2	1	0.16
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE3	1	0.16
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE1	1	0.16
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE2	1	0.16
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE3	1	0.16
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE1	1	0.16
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE2	1	0.16
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE3	1	0.16
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	4	0.16
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	4	0.16
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	4	0.16
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	4	0.16
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	4	0.16
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	4	0.16
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	4	0.16
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	4	0.16
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	4	0.16
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	8	0.16
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	8	0.16
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	8	0.16
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	8	0.16
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	8	0.16
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	8	0.16
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	8	0.16
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	8	0.16
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	8	0.16
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	5	0.16
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	5	0.16
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	5	0.16
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	5	0.16
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	5	0.16
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	5	0.16
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	5	0.16
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	5	0.16
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	5	0.16
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	3	0.16
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	3	0.16
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	3	0.16
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	3	0.16
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	3	0.16
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	3	0.16
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	3	0.16
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	3	0.16
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD11	2	0.16
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD12	2	0.16
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD13	2	0.16
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD11	2	0.16
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD12	2	0.16
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD13	2	0.16
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD11	2	0.16
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD12	2	0.16
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD13	2	0.16
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	10	0.16
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	10	0.16
(1,449)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	10	0.16
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	10	0.16
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	10	0.16
(1,449)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	10	0.16
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	10	0.16
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	10	0.16
(1,449)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	10	0.16
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD11	6	0.16
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD12	6	0.16
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD13	6	0.16
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD11	6	0.16
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD12	6	0.16
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD13	6	0.16
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD11	6	0.16
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD12	6	0.16
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD13	6	0.16
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	9	0.16
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	9	0.16
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	9	0.16
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	9	0.16
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	9	0.16
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	9	0.16
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	9	0.16
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	9	0.16
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	9	0.16
(1,418)	1:32:A:LEU:HD11	1:119:A:MET:HE1	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:32:A:LEU:HD11	1:119:A:MET:HE2	7	0.16
(1,418)	1:32:A:LEU:HD11	1:119:A:MET:HE3	7	0.16
(1,418)	1:32:A:LEU:HD12	1:119:A:MET:HE1	7	0.16
(1,418)	1:32:A:LEU:HD12	1:119:A:MET:HE2	7	0.16
(1,418)	1:32:A:LEU:HD12	1:119:A:MET:HE3	7	0.16
(1,418)	1:32:A:LEU:HD13	1:119:A:MET:HE1	7	0.16
(1,418)	1:32:A:LEU:HD13	1:119:A:MET:HE2	7	0.16
(1,418)	1:32:A:LEU:HD13	1:119:A:MET:HE3	7	0.16
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB1	6	0.16
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB2	6	0.16
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB3	6	0.16
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB1	6	0.16
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB2	6	0.16
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB3	6	0.16
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB1	6	0.16
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB2	6	0.16
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB3	6	0.16
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	4	0.16
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	4	0.16
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	4	0.16
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	4	0.16
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	4	0.16
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	4	0.16
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	4	0.16
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	4	0.16
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	4	0.16
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	9	0.16
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	9	0.16
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	9	0.16
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	9	0.16
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	9	0.16
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	9	0.16
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	9	0.16
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	9	0.16
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	9	0.16
(1,336)	1:93:A:ASP:H	1:186:A:VAL:H	4	0.16
(1,314)	1:58:A:LYS:H	1:96:A:ILE:H	2	0.16
(1,288)	1:196:A:GLU:H	1:199:A:GLU:H	4	0.16
(1,116)	1:176:A:THR:H	1:177:A:GLY:H	7	0.16
(1,109)	1:167:A:GLY:H	1:168:A:GLY:H	3	0.16
(1,107)	1:165:A:SER:H	1:166:A:ALA:H	2	0.16
(1,61)	1:94:A:THR:H	1:95:A:GLY:H	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,144)	1:208:A:LYS:H	1:204:A:LYS:O	9	0.15
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	1	0.15
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	8	0.15
(1,1114)	1:133:A:GLN:HE22	1:130:A:MET:HE1	4	0.15
(1,1114)	1:133:A:GLN:HE22	1:130:A:MET:HE2	4	0.15
(1,1114)	1:133:A:GLN:HE22	1:130:A:MET:HE3	4	0.15
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG11	5	0.15
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG12	5	0.15
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG13	5	0.15
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD11	2	0.15
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD12	2	0.15
(1,1079)	1:213:A:PHE:H	1:218:A:ILE:HD13	2	0.15
(1,1078)	1:213:A:PHE:H	1:214:A:ILE:HD11	7	0.15
(1,1078)	1:213:A:PHE:H	1:214:A:ILE:HD12	7	0.15
(1,1078)	1:213:A:PHE:H	1:214:A:ILE:HD13	7	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	3	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	3	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	3	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	5	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	5	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	5	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	9	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	9	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	9	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	10	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	10	0.15
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	10	0.15
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD11	3	0.15
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD12	3	0.15
(1,1066)	1:207:A:VAL:H	1:49:A:ILE:HD13	3	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD21	7	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD22	7	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD23	7	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD21	8	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD22	8	0.15
(1,1053)	1:203:A:ILE:H	1:220:A:LEU:HD23	8	0.15
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD21	4	0.15
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD22	4	0.15
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD23	4	0.15
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG21	9	0.15
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG22	9	0.15
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG23	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:188:A:LEU:H	1:145:A:ALA:HB1	9	0.15
(1,1008)	1:188:A:LEU:H	1:145:A:ALA:HB2	9	0.15
(1,1008)	1:188:A:LEU:H	1:145:A:ALA:HB3	9	0.15
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG21	5	0.15
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG22	5	0.15
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG23	5	0.15
(1,966)	1:170:A:PHE:H	1:171:A:THR:HG21	9	0.15
(1,966)	1:170:A:PHE:H	1:171:A:THR:HG22	9	0.15
(1,966)	1:170:A:PHE:H	1:171:A:THR:HG23	9	0.15
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	6	0.15
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	6	0.15
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	6	0.15
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB1	1	0.15
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB2	1	0.15
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB3	1	0.15
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG21	3	0.15
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG22	3	0.15
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG23	3	0.15
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG21	1	0.15
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG22	1	0.15
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG23	1	0.15
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD11	1	0.15
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD12	1	0.15
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD13	1	0.15
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD11	4	0.15
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD12	4	0.15
(1,876)	1:127:A:ASP:H	1:122:A:LEU:HD13	4	0.15
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD11	2	0.15
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD12	2	0.15
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD13	2	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD21	2	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD22	2	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD23	2	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD21	7	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD22	7	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD23	7	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD21	8	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD22	8	0.15
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD23	8	0.15
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB1	5	0.15
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB2	5	0.15
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD11	5	0.15
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD12	5	0.15
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD13	5	0.15
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE1	5	0.15
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE2	5	0.15
(1,834)	1:93:A:ASP:H	1:180:A:MET:HE3	5	0.15
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	1	0.15
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	1	0.15
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	1	0.15
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	10	0.15
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	10	0.15
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	10	0.15
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	6	0.15
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	6	0.15
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	6	0.15
(1,824)	1:91:A:ILE:H	1:186:A:VAL:HG21	4	0.15
(1,824)	1:91:A:ILE:H	1:186:A:VAL:HG22	4	0.15
(1,824)	1:91:A:ILE:H	1:186:A:VAL:HG23	4	0.15
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	10	0.15
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	10	0.15
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	10	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG21	3	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG22	3	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG23	3	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG21	7	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG22	7	0.15
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG23	7	0.15
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD21	2	0.15
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD22	2	0.15
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD23	2	0.15
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD11	9	0.15
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD12	9	0.15
(1,711)	1:43:A:ILE:H	1:143:A:LEU:HD13	9	0.15
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	3	0.15
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	3	0.15
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	3	0.15
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD11	3	0.15
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD12	3	0.15
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD13	3	0.15
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB1	3	0.15
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB2	3	0.15
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:31:A:SER:H	1:30:A:MET:HE1	1	0.15
(1,693)	1:31:A:SER:H	1:30:A:MET:HE2	1	0.15
(1,693)	1:31:A:SER:H	1:30:A:MET:HE3	1	0.15
(1,691)	1:29:A:LEU:H	1:115:A:THR:HG21	5	0.15
(1,691)	1:29:A:LEU:H	1:115:A:THR:HG22	5	0.15
(1,691)	1:29:A:LEU:H	1:115:A:THR:HG23	5	0.15
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB1	7	0.15
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB2	7	0.15
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB3	7	0.15
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	6	0.15
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	6	0.15
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	6	0.15
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB1	3	0.15
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB2	3	0.15
(1,683)	1:26:A:ILE:H	1:24:A:ALA:HB3	3	0.15
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG11	7	0.15
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG12	7	0.15
(1,668)	1:222:A:VAL:H	1:222:A:VAL:HG13	7	0.15
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG21	2	0.15
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG22	2	0.15
(1,663)	1:207:A:VAL:H	1:207:A:VAL:HG23	2	0.15
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	7	0.15
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	7	0.15
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	7	0.15
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD11	6	0.15
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD12	6	0.15
(1,617)	1:76:A:LEU:H	1:76:A:LEU:HD13	6	0.15
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD11	6	0.15
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD12	6	0.15
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD13	6	0.15
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG21	5	0.15
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG22	5	0.15
(1,598)	1:17:A:VAL:H	1:17:A:VAL:HG23	5	0.15
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD11	7	0.15
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD12	7	0.15
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD13	7	0.15
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD11	7	0.15
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD12	7	0.15
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD13	7	0.15
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD11	7	0.15
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD12	7	0.15
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD13	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	8	0.15
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	8	0.15
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	8	0.15
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	8	0.15
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	8	0.15
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	8	0.15
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	8	0.15
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	8	0.15
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	8	0.15
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	6	0.15
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	6	0.15
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	6	0.15
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	6	0.15
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	6	0.15
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	6	0.15
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	6	0.15
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	6	0.15
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	6	0.15
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	9	0.15
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	9	0.15
(1,541)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	9	0.15
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	9	0.15
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	9	0.15
(1,541)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	9	0.15
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	9	0.15
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	9	0.15
(1,541)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	9	0.15
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG11	5	0.15
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG12	5	0.15
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG13	5	0.15
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG11	5	0.15
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG12	5	0.15
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG13	5	0.15
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG11	5	0.15
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG12	5	0.15
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG13	5	0.15
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG11	2	0.15
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG12	2	0.15
(1,532)	1:107:A:LEU:HD11	1:150:A:VAL:HG13	2	0.15
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG11	2	0.15
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG12	2	0.15
(1,532)	1:107:A:LEU:HD12	1:150:A:VAL:HG13	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG11	2	0.15
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG12	2	0.15
(1,532)	1:107:A:LEU:HD13	1:150:A:VAL:HG13	2	0.15
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	7	0.15
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	7	0.15
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	7	0.15
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	7	0.15
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	7	0.15
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	7	0.15
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	7	0.15
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	7	0.15
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	7	0.15
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG11	9	0.15
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG12	9	0.15
(1,513)	1:98:A:MET:HE1	1:150:A:VAL:HG13	9	0.15
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG11	9	0.15
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG12	9	0.15
(1,513)	1:98:A:MET:HE2	1:150:A:VAL:HG13	9	0.15
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG11	9	0.15
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG12	9	0.15
(1,513)	1:98:A:MET:HE3	1:150:A:VAL:HG13	9	0.15
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	4	0.15
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	4	0.15
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	4	0.15
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	4	0.15
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	4	0.15
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	4	0.15
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	4	0.15
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	4	0.15
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	4	0.15
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	8	0.15
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	8	0.15
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	8	0.15
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	8	0.15
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	8	0.15
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	8	0.15
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	8	0.15
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	8	0.15
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	8	0.15
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	3	0.15
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	3	0.15
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	3	0.15
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	3	0.15
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	3	0.15
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	3	0.15
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	3	0.15
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	3	0.15
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG21	8	0.15
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG22	8	0.15
(1,487)	1:81:A:ILE:HD11	1:90:A:THR:HG23	8	0.15
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG21	8	0.15
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG22	8	0.15
(1,487)	1:81:A:ILE:HD12	1:90:A:THR:HG23	8	0.15
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG21	8	0.15
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG22	8	0.15
(1,487)	1:81:A:ILE:HD13	1:90:A:THR:HG23	8	0.15
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	9	0.15
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	9	0.15
(1,483)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	9	0.15
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	9	0.15
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	9	0.15
(1,483)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	9	0.15
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	9	0.15
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	9	0.15
(1,483)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	9	0.15
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	2	0.15
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	2	0.15
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	2	0.15
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	2	0.15
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	2	0.15
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	2	0.15
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	2	0.15
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	2	0.15
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	2	0.15
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	2	0.15
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	2	0.15
(1,465)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	2	0.15
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	2	0.15
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	2	0.15
(1,465)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	2	0.15
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	2	0.15
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	2	0.15
(1,465)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	6	0.15
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	6	0.15
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	6	0.15
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	6	0.15
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	6	0.15
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	6	0.15
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	6	0.15
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	6	0.15
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	6	0.15
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	8	0.15
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	8	0.15
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	8	0.15
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	8	0.15
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	8	0.15
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	8	0.15
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	8	0.15
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	8	0.15
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	8	0.15
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	10	0.15
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	10	0.15
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	10	0.15
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	10	0.15
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	10	0.15
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	10	0.15
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	10	0.15
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	10	0.15
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	10	0.15
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB1	8	0.15
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB2	8	0.15
(1,417)	1:30:A:MET:HE1	1:166:A:ALA:HB3	8	0.15
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB1	8	0.15
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB2	8	0.15
(1,417)	1:30:A:MET:HE2	1:166:A:ALA:HB3	8	0.15
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB1	8	0.15
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB2	8	0.15
(1,417)	1:30:A:MET:HE3	1:166:A:ALA:HB3	8	0.15
(1,416)	1:30:A:MET:HE1	1:34:A:ILE:HD11	10	0.15
(1,416)	1:30:A:MET:HE1	1:34:A:ILE:HD12	10	0.15
(1,416)	1:30:A:MET:HE1	1:34:A:ILE:HD13	10	0.15
(1,416)	1:30:A:MET:HE2	1:34:A:ILE:HD11	10	0.15
(1,416)	1:30:A:MET:HE2	1:34:A:ILE:HD12	10	0.15
(1,416)	1:30:A:MET:HE2	1:34:A:ILE:HD13	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:30:A:MET:HE3	1:34:A:ILE:HD11	10	0.15
(1,416)	1:30:A:MET:HE3	1:34:A:ILE:HD12	10	0.15
(1,416)	1:30:A:MET:HE3	1:34:A:ILE:HD13	10	0.15
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	2	0.15
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	2	0.15
(1,410)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	2	0.15
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	2	0.15
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	2	0.15
(1,410)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	2	0.15
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	2	0.15
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	2	0.15
(1,410)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	2	0.15
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	3	0.15
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	3	0.15
(1,405)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	3	0.15
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	3	0.15
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	3	0.15
(1,405)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	3	0.15
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	3	0.15
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	3	0.15
(1,405)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	3	0.15
(1,339)	1:122:A:LEU:H	1:126:A:ALA:H	9	0.15
(1,337)	1:103:A:LEU:H	1:107:A:LEU:H	9	0.15
(1,277)	1:131:A:ILE:H	1:134:A:PHE:H	1	0.15
(1,263)	1:69:A:LYS:H	1:72:A:SER:H	7	0.15
(1,199)	1:95:A:GLY:H	1:97:A:GLY:H	2	0.15
(1,116)	1:176:A:THR:H	1:177:A:GLY:H	3	0.15
(1,110)	1:168:A:GLY:H	1:169:A:SER:H	3	0.15
(1,47)	1:76:A:LEU:H	1:77:A:HIS:H	3	0.15
(1,40)	1:68:A:SER:H	1:69:A:LYS:H	8	0.15
(2,98)	1:44:A:PHE:H	1:41:A:LYS:O	2	0.14
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	1	0.14
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG11	8	0.14
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG12	8	0.14
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG13	8	0.14
(1,1085)	1:218:A:ILE:H	1:78:A:ILE:HD11	10	0.14
(1,1085)	1:218:A:ILE:H	1:78:A:ILE:HD12	10	0.14
(1,1085)	1:218:A:ILE:H	1:78:A:ILE:HD13	10	0.14
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD11	6	0.14
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD12	6	0.14
(1,1083)	1:216:A:TYR:H	1:214:A:ILE:HD13	6	0.14
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG21	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG22	3	0.14
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG23	3	0.14
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG21	10	0.14
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG22	10	0.14
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG23	10	0.14
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD11	5	0.14
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD12	5	0.14
(1,1056)	1:204:A:LYS:H	1:206:A:ILE:HD13	5	0.14
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG21	4	0.14
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG22	4	0.14
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG23	4	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD11	6	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD12	6	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD13	6	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD11	10	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD12	10	0.14
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD13	10	0.14
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG21	3	0.14
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG22	3	0.14
(1,1031)	1:196:A:GLU:H	1:195:A:THR:HG23	3	0.14
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB1	9	0.14
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB2	9	0.14
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB3	9	0.14
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG21	1	0.14
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG22	1	0.14
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG23	1	0.14
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG21	10	0.14
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG22	10	0.14
(1,1019)	1:190:A:LEU:H	1:88:A:THR:HG23	10	0.14
(1,1005)	1:188:A:LEU:H	1:89:A:LEU:HD21	4	0.14
(1,1005)	1:188:A:LEU:H	1:89:A:LEU:HD22	4	0.14
(1,1005)	1:188:A:LEU:H	1:89:A:LEU:HD23	4	0.14
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	2	0.14
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	2	0.14
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	2	0.14
(1,983)	1:185:A:LYS:H	1:98:A:MET:HE1	8	0.14
(1,983)	1:185:A:LYS:H	1:98:A:MET:HE2	8	0.14
(1,983)	1:185:A:LYS:H	1:98:A:MET:HE3	8	0.14
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	1	0.14
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	1	0.14
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	1	0.14
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG11	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG12	10	0.14
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG13	10	0.14
(1,956)	1:162:A:TRP:H	1:172:A:VAL:HG21	7	0.14
(1,956)	1:162:A:TRP:H	1:172:A:VAL:HG22	7	0.14
(1,956)	1:162:A:TRP:H	1:172:A:VAL:HG23	7	0.14
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	7	0.14
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	7	0.14
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	7	0.14
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG21	9	0.14
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG22	9	0.14
(1,942)	1:159:A:GLN:H	1:174:A:THR:HG23	9	0.14
(1,939)	1:152:A:THR:H	1:184:A:THR:HG21	1	0.14
(1,939)	1:152:A:THR:H	1:184:A:THR:HG22	1	0.14
(1,939)	1:152:A:THR:H	1:184:A:THR:HG23	1	0.14
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG21	5	0.14
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG22	5	0.14
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG23	5	0.14
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE1	2	0.14
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE2	2	0.14
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE3	2	0.14
(1,902)	1:142:A:TYR:H	1:141:A:ALA:HB1	3	0.14
(1,902)	1:142:A:TYR:H	1:141:A:ALA:HB2	3	0.14
(1,902)	1:142:A:TYR:H	1:141:A:ALA:HB3	3	0.14
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG21	7	0.14
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG22	7	0.14
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG23	7	0.14
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD11	1	0.14
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD12	1	0.14
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD13	1	0.14
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG11	6	0.14
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG12	6	0.14
(1,886)	1:137:A:GLY:H	1:136:A:VAL:HG13	6	0.14
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB1	8	0.14
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB2	8	0.14
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB3	8	0.14
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD11	3	0.14
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD12	3	0.14
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD13	3	0.14
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG11	3	0.14
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG12	3	0.14
(1,848)	1:104:A:ILE:H	1:172:A:VAL:HG13	3	0.14
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	5	0.14
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	5	0.14
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG21	2	0.14
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG22	2	0.14
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG23	2	0.14
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG21	10	0.14
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG22	10	0.14
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG23	10	0.14
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD11	7	0.14
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD12	7	0.14
(1,777)	1:78:A:ILE:H	1:56:A:LEU:HD13	7	0.14
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD11	1	0.14
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD12	1	0.14
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD13	1	0.14
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	8	0.14
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	8	0.14
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	8	0.14
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	6	0.14
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	6	0.14
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	6	0.14
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	9	0.14
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	9	0.14
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	9	0.14
(1,693)	1:31:A:SER:H	1:30:A:MET:HE1	8	0.14
(1,693)	1:31:A:SER:H	1:30:A:MET:HE2	8	0.14
(1,693)	1:31:A:SER:H	1:30:A:MET:HE3	8	0.14
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	1	0.14
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	1	0.14
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	1	0.14
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	10	0.14
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	10	0.14
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	10	0.14
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD11	8	0.14
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD12	8	0.14
(1,586)	1:195:A:THR:HG21	1:198:A:LEU:HD13	8	0.14
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD11	8	0.14
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD12	8	0.14
(1,586)	1:195:A:THR:HG22	1:198:A:LEU:HD13	8	0.14
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD11	8	0.14
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD12	8	0.14
(1,586)	1:195:A:THR:HG23	1:198:A:LEU:HD13	8	0.14
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD21	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD22	3	0.14
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD23	3	0.14
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD21	3	0.14
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD22	3	0.14
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD23	3	0.14
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD21	3	0.14
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD22	3	0.14
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD23	3	0.14
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	5	0.14
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	5	0.14
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	5	0.14
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	5	0.14
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	5	0.14
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	5	0.14
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	5	0.14
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	5	0.14
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	5	0.14
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD11	9	0.14
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD12	9	0.14
(1,566)	1:149:A:THR:HG21	1:187:A:ILE:HD13	9	0.14
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD11	9	0.14
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD12	9	0.14
(1,566)	1:149:A:THR:HG22	1:187:A:ILE:HD13	9	0.14
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD11	9	0.14
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD12	9	0.14
(1,566)	1:149:A:THR:HG23	1:187:A:ILE:HD13	9	0.14
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	8	0.14
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	8	0.14
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	8	0.14
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	8	0.14
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	8	0.14
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	8	0.14
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	8	0.14
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	8	0.14
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	8	0.14
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE1	8	0.14
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE2	8	0.14
(1,546)	1:126:A:ALA:HB1	1:130:A:MET:HE3	8	0.14
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE1	8	0.14
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE2	8	0.14
(1,546)	1:126:A:ALA:HB2	1:130:A:MET:HE3	8	0.14
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE1	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE2	8	0.14
(1,546)	1:126:A:ALA:HB3	1:130:A:MET:HE3	8	0.14
(1,537)	1:115:A:THR:HG21	1:136:A:VAL:HG11	6	0.14
(1,537)	1:115:A:THR:HG21	1:136:A:VAL:HG12	6	0.14
(1,537)	1:115:A:THR:HG21	1:136:A:VAL:HG13	6	0.14
(1,537)	1:115:A:THR:HG22	1:136:A:VAL:HG11	6	0.14
(1,537)	1:115:A:THR:HG22	1:136:A:VAL:HG12	6	0.14
(1,537)	1:115:A:THR:HG22	1:136:A:VAL:HG13	6	0.14
(1,537)	1:115:A:THR:HG23	1:136:A:VAL:HG11	6	0.14
(1,537)	1:115:A:THR:HG23	1:136:A:VAL:HG12	6	0.14
(1,537)	1:115:A:THR:HG23	1:136:A:VAL:HG13	6	0.14
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG11	6	0.14
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG12	6	0.14
(1,533)	1:107:A:LEU:HD21	1:150:A:VAL:HG13	6	0.14
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG11	6	0.14
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG12	6	0.14
(1,533)	1:107:A:LEU:HD22	1:150:A:VAL:HG13	6	0.14
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG11	6	0.14
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG12	6	0.14
(1,533)	1:107:A:LEU:HD23	1:150:A:VAL:HG13	6	0.14
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG21	8	0.14
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG22	8	0.14
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG23	8	0.14
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG21	8	0.14
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG22	8	0.14
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG23	8	0.14
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG21	8	0.14
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG22	8	0.14
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG23	8	0.14
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB1	6	0.14
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB2	6	0.14
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB3	6	0.14
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB1	6	0.14
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB2	6	0.14
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB3	6	0.14
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB1	6	0.14
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB2	6	0.14
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB3	6	0.14
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD21	2	0.14
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD22	2	0.14
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD23	2	0.14
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD21	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD22	2	0.14
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD23	2	0.14
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD21	2	0.14
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD22	2	0.14
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD23	2	0.14
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE1	4	0.14
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE2	4	0.14
(1,507)	1:92:A:VAL:HG21	1:180:A:MET:HE3	4	0.14
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE1	4	0.14
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE2	4	0.14
(1,507)	1:92:A:VAL:HG22	1:180:A:MET:HE3	4	0.14
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE1	4	0.14
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE2	4	0.14
(1,507)	1:92:A:VAL:HG23	1:180:A:MET:HE3	4	0.14
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	5	0.14
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	5	0.14
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	5	0.14
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	5	0.14
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	5	0.14
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	5	0.14
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	5	0.14
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	5	0.14
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	5	0.14
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	9	0.14
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	9	0.14
(1,494)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	9	0.14
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	9	0.14
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	9	0.14
(1,494)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	9	0.14
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	9	0.14
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	9	0.14
(1,494)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	9	0.14
(1,491)	1:89:A:LEU:HD11	1:198:A:LEU:HD21	7	0.14
(1,491)	1:89:A:LEU:HD11	1:198:A:LEU:HD22	7	0.14
(1,491)	1:89:A:LEU:HD11	1:198:A:LEU:HD23	7	0.14
(1,491)	1:89:A:LEU:HD12	1:198:A:LEU:HD21	7	0.14
(1,491)	1:89:A:LEU:HD12	1:198:A:LEU:HD22	7	0.14
(1,491)	1:89:A:LEU:HD12	1:198:A:LEU:HD23	7	0.14
(1,491)	1:89:A:LEU:HD13	1:198:A:LEU:HD21	7	0.14
(1,491)	1:89:A:LEU:HD13	1:198:A:LEU:HD22	7	0.14
(1,491)	1:89:A:LEU:HD13	1:198:A:LEU:HD23	7	0.14
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	3	0.14
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	3	0.14
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	3	0.14
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	3	0.14
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	3	0.14
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	3	0.14
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	3	0.14
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	3	0.14
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	5	0.14
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	5	0.14
(1,474)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	5	0.14
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	5	0.14
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	5	0.14
(1,474)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	5	0.14
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	5	0.14
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	5	0.14
(1,474)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	5	0.14
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	4	0.14
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	4	0.14
(1,440)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	4	0.14
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	4	0.14
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	4	0.14
(1,440)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	4	0.14
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	4	0.14
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	4	0.14
(1,440)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	4	0.14
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD21	9	0.14
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD22	9	0.14
(1,432)	1:43:A:ILE:HD11	1:143:A:LEU:HD23	9	0.14
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD21	9	0.14
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD22	9	0.14
(1,432)	1:43:A:ILE:HD12	1:143:A:LEU:HD23	9	0.14
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD21	9	0.14
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD22	9	0.14
(1,432)	1:43:A:ILE:HD13	1:143:A:LEU:HD23	9	0.14
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	2	0.14
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	2	0.14
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	2	0.14
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	2	0.14
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	2	0.14
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	2	0.14
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	2	0.14
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	2	0.14
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	1	0.14
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	1	0.14
(1,397)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	1	0.14
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	1	0.14
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	1	0.14
(1,397)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	1	0.14
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	1	0.14
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	1	0.14
(1,397)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	1	0.14
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	7	0.14
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	7	0.14
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	7	0.14
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	7	0.14
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	7	0.14
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	7	0.14
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	7	0.14
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	7	0.14
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	7	0.14
(1,325)	1:80:A:LEU:H	1:221:A:PHE:H	1	0.14
(1,287)	1:194:A:GLN:H	1:197:A:TYR:H	9	0.14
(1,277)	1:131:A:ILE:H	1:134:A:PHE:H	7	0.14
(1,276)	1:128:A:ILE:H	1:131:A:ILE:H	2	0.14
(1,220)	1:167:A:GLY:H	1:169:A:SER:H	4	0.14
(1,208)	1:123:A:GLN:H	1:125:A:GLY:H	3	0.14
(1,193)	1:72:A:SER:H	1:74:A:LYS:H	1	0.14
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	5	0.13
(2,40)	1:93:A:ASP:H	1:184:A:THR:O	1	0.13
(1,1113)	1:133:A:GLN:HE21	1:130:A:MET:HE1	5	0.13
(1,1113)	1:133:A:GLN:HE21	1:130:A:MET:HE2	5	0.13
(1,1113)	1:133:A:GLN:HE21	1:130:A:MET:HE3	5	0.13
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG21	6	0.13
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG22	6	0.13
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG23	6	0.13
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD11	1	0.13
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD12	1	0.13
(1,1068)	1:207:A:VAL:H	1:206:A:ILE:HD13	1	0.13
(1,1055)	1:204:A:LYS:H	1:203:A:ILE:HD11	10	0.13
(1,1055)	1:204:A:LYS:H	1:203:A:ILE:HD12	10	0.13
(1,1055)	1:204:A:LYS:H	1:203:A:ILE:HD13	10	0.13
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD12	10	0.13
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD13	10	0.13
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD21	4	0.13
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD22	4	0.13
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD23	4	0.13
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG21	1	0.13
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG22	1	0.13
(1,1046)	1:200:A:GLU:H	1:222:A:VAL:HG23	1	0.13
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD21	2	0.13
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD22	2	0.13
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD23	2	0.13
(1,1038)	1:198:A:LEU:H	1:190:A:LEU:HD11	5	0.13
(1,1038)	1:198:A:LEU:H	1:190:A:LEU:HD12	5	0.13
(1,1038)	1:198:A:LEU:H	1:190:A:LEU:HD13	5	0.13
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD11	5	0.13
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD12	5	0.13
(1,1036)	1:197:A:TYR:H	1:198:A:LEU:HD13	5	0.13
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD21	3	0.13
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD22	3	0.13
(1,1034)	1:197:A:TYR:H	1:190:A:LEU:HD23	3	0.13
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG21	7	0.13
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG22	7	0.13
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG23	7	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	5	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	5	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	5	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	8	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	8	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	8	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	9	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	9	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	9	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	10	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	10	0.13
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	10	0.13
(1,981)	1:185:A:LYS:H	1:92:A:VAL:HG11	4	0.13
(1,981)	1:185:A:LYS:H	1:92:A:VAL:HG12	4	0.13
(1,981)	1:185:A:LYS:H	1:92:A:VAL:HG13	4	0.13
(1,976)	1:175:A:ASP:H	1:176:A:THR:HG21	10	0.13
(1,976)	1:175:A:ASP:H	1:176:A:THR:HG22	10	0.13
(1,976)	1:175:A:ASP:H	1:176:A:THR:HG23	10	0.13
(1,958)	1:163:A:GLU:H	1:161:A:ALA:HB1	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:163:A:GLU:H	1:161:A:ALA:HB2	6	0.13
(1,958)	1:163:A:GLU:H	1:161:A:ALA:HB3	6	0.13
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	7	0.13
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	7	0.13
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	7	0.13
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	2	0.13
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	2	0.13
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	2	0.13
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE1	7	0.13
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE2	7	0.13
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE3	7	0.13
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG21	1	0.13
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG22	1	0.13
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG23	1	0.13
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG21	10	0.13
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG22	10	0.13
(1,934)	1:151:A:ILE:H	1:150:A:VAL:HG23	10	0.13
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG21	7	0.13
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG22	7	0.13
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG23	7	0.13
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG21	3	0.13
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG22	3	0.13
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG23	3	0.13
(1,903)	1:142:A:TYR:H	1:143:A:LEU:HD11	10	0.13
(1,903)	1:142:A:TYR:H	1:143:A:LEU:HD12	10	0.13
(1,903)	1:142:A:TYR:H	1:143:A:LEU:HD13	10	0.13
(1,901)	1:142:A:TYR:H	1:33:A:ILE:HD11	2	0.13
(1,901)	1:142:A:TYR:H	1:33:A:ILE:HD12	2	0.13
(1,901)	1:142:A:TYR:H	1:33:A:ILE:HD13	2	0.13
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD11	8	0.13
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD12	8	0.13
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD13	8	0.13
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG21	6	0.13
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG22	6	0.13
(1,896)	1:139:A:TYR:H	1:136:A:VAL:HG23	6	0.13
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD11	4	0.13
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD12	4	0.13
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD13	4	0.13
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD11	6	0.13
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD12	6	0.13
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD13	6	0.13
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB1	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB2	4	0.13
(1,877)	1:127:A:ASP:H	1:126:A:ALA:HB3	4	0.13
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG21	1	0.13
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG22	1	0.13
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG23	1	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD11	4	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD12	4	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD13	4	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD11	8	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD12	8	0.13
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD13	8	0.13
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD21	1	0.13
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD22	1	0.13
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD23	1	0.13
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD21	9	0.13
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD22	9	0.13
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD23	9	0.13
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG21	4	0.13
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG22	4	0.13
(1,787)	1:80:A:LEU:H	1:219:A:THR:HG23	4	0.13
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD21	4	0.13
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD22	4	0.13
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD23	4	0.13
(1,778)	1:78:A:ILE:H	1:56:A:LEU:HD21	8	0.13
(1,778)	1:78:A:ILE:H	1:56:A:LEU:HD22	8	0.13
(1,778)	1:78:A:ILE:H	1:56:A:LEU:HD23	8	0.13
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	7	0.13
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	7	0.13
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	7	0.13
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD11	2	0.13
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD12	2	0.13
(1,696)	1:32:A:LEU:H	1:29:A:LEU:HD13	2	0.13
(1,665)	1:218:A:ILE:H	1:218:A:ILE:HD11	4	0.13
(1,665)	1:218:A:ILE:H	1:218:A:ILE:HD12	4	0.13
(1,665)	1:218:A:ILE:H	1:218:A:ILE:HD13	4	0.13
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD11	8	0.13
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD12	8	0.13
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD13	8	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	2	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	2	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	2	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	5	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	5	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG21	8	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG22	8	0.13
(1,643)	1:144:A:VAL:H	1:144:A:VAL:HG23	8	0.13
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD11	3	0.13
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD12	3	0.13
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD13	3	0.13
(1,618)	1:76:A:LEU:H	1:76:A:LEU:HD21	3	0.13
(1,618)	1:76:A:LEU:H	1:76:A:LEU:HD22	3	0.13
(1,618)	1:76:A:LEU:H	1:76:A:LEU:HD23	3	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD11	1	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD12	1	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD13	1	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD11	7	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD12	7	0.13
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD13	7	0.13
(1,594)	1:220:A:LEU:HD11	1:222:A:VAL:HG21	5	0.13
(1,594)	1:220:A:LEU:HD11	1:222:A:VAL:HG22	5	0.13
(1,594)	1:220:A:LEU:HD11	1:222:A:VAL:HG23	5	0.13
(1,594)	1:220:A:LEU:HD12	1:222:A:VAL:HG21	5	0.13
(1,594)	1:220:A:LEU:HD12	1:222:A:VAL:HG22	5	0.13
(1,594)	1:220:A:LEU:HD12	1:222:A:VAL:HG23	5	0.13
(1,594)	1:220:A:LEU:HD13	1:222:A:VAL:HG21	5	0.13
(1,594)	1:220:A:LEU:HD13	1:222:A:VAL:HG22	5	0.13
(1,594)	1:220:A:LEU:HD13	1:222:A:VAL:HG23	5	0.13
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	1	0.13
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	1	0.13
(1,562)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	1	0.13
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	1	0.13
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	1	0.13
(1,562)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	1	0.13
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	1	0.13
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	1	0.13
(1,562)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	1	0.13
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	1	0.13
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	1	0.13
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	1	0.13
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	1	0.13
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	1	0.13
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	1	0.13
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	1	0.13
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	1	0.13
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE1	2	0.13
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE2	2	0.13
(1,542)	1:121:A:ALA:HB1	1:130:A:MET:HE3	2	0.13
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE1	2	0.13
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE2	2	0.13
(1,542)	1:121:A:ALA:HB2	1:130:A:MET:HE3	2	0.13
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE1	2	0.13
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE2	2	0.13
(1,542)	1:121:A:ALA:HB3	1:130:A:MET:HE3	2	0.13
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG21	9	0.13
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG22	9	0.13
(1,529)	1:103:A:LEU:HD21	1:172:A:VAL:HG23	9	0.13
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG21	9	0.13
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG22	9	0.13
(1,529)	1:103:A:LEU:HD22	1:172:A:VAL:HG23	9	0.13
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG21	9	0.13
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG22	9	0.13
(1,529)	1:103:A:LEU:HD23	1:172:A:VAL:HG23	9	0.13
(1,528)	1:103:A:LEU:HD21	1:172:A:VAL:HG11	3	0.13
(1,528)	1:103:A:LEU:HD21	1:172:A:VAL:HG12	3	0.13
(1,528)	1:103:A:LEU:HD21	1:172:A:VAL:HG13	3	0.13
(1,528)	1:103:A:LEU:HD22	1:172:A:VAL:HG11	3	0.13
(1,528)	1:103:A:LEU:HD22	1:172:A:VAL:HG12	3	0.13
(1,528)	1:103:A:LEU:HD22	1:172:A:VAL:HG13	3	0.13
(1,528)	1:103:A:LEU:HD23	1:172:A:VAL:HG11	3	0.13
(1,528)	1:103:A:LEU:HD23	1:172:A:VAL:HG12	3	0.13
(1,528)	1:103:A:LEU:HD23	1:172:A:VAL:HG13	3	0.13
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	5	0.13
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	5	0.13
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	5	0.13
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	5	0.13
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	5	0.13
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	5	0.13
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	5	0.13
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	5	0.13
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	5	0.13
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	8	0.13
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	8	0.13
(1,526)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	8	0.13
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	8	0.13
(1,526)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	8	0.13
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	8	0.13
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	8	0.13
(1,526)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	8	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	1	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	1	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	1	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	1	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	1	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	1	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	1	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	1	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	1	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	6	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	6	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	6	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	6	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	6	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	6	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	6	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	6	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	6	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	9	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	9	0.13
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	9	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	9	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	9	0.13
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	9	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	9	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	9	0.13
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	9	0.13
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	3	0.13
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	3	0.13
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	3	0.13
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	3	0.13
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	3	0.13
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	3	0.13
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	3	0.13
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	3	0.13
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	3	0.13
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	7	0.13
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	7	0.13
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	7	0.13
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	7	0.13
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	7	0.13
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	7	0.13
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	7	0.13
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	7	0.13
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	7	0.13
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	7	0.13
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	7	0.13
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	7	0.13
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	7	0.13
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	7	0.13
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	7	0.13
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	7	0.13
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	7	0.13
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD11	5	0.13
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD12	5	0.13
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD13	5	0.13
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD11	5	0.13
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD12	5	0.13
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD13	5	0.13
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD11	5	0.13
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD12	5	0.13
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD13	5	0.13
(1,488)	1:81:A:ILE:HD11	1:92:A:VAL:HG11	7	0.13
(1,488)	1:81:A:ILE:HD11	1:92:A:VAL:HG12	7	0.13
(1,488)	1:81:A:ILE:HD11	1:92:A:VAL:HG13	7	0.13
(1,488)	1:81:A:ILE:HD12	1:92:A:VAL:HG11	7	0.13
(1,488)	1:81:A:ILE:HD12	1:92:A:VAL:HG12	7	0.13
(1,488)	1:81:A:ILE:HD12	1:92:A:VAL:HG13	7	0.13
(1,488)	1:81:A:ILE:HD13	1:92:A:VAL:HG11	7	0.13
(1,488)	1:81:A:ILE:HD13	1:92:A:VAL:HG12	7	0.13
(1,488)	1:81:A:ILE:HD13	1:92:A:VAL:HG13	7	0.13
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	1	0.13
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	1	0.13
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	1	0.13
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	1	0.13
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	1	0.13
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	1	0.13
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	1	0.13
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	1	0.13
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	5	0.13
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	5	0.13
(1,481)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	5	0.13
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	5	0.13
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	5	0.13
(1,481)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	5	0.13
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	5	0.13
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	5	0.13
(1,481)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	5	0.13
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD11	10	0.13
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD12	10	0.13
(1,459)	1:48:A:LEU:HD21	1:188:A:LEU:HD13	10	0.13
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD11	10	0.13
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD12	10	0.13
(1,459)	1:48:A:LEU:HD22	1:188:A:LEU:HD13	10	0.13
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD11	10	0.13
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD12	10	0.13
(1,459)	1:48:A:LEU:HD23	1:188:A:LEU:HD13	10	0.13
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	5	0.13
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	5	0.13
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	5	0.13
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	5	0.13
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	5	0.13
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	5	0.13
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	5	0.13
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	5	0.13
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	5	0.13
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD21	4	0.13
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD22	4	0.13
(1,445)	1:45:A:LEU:HD21	1:80:A:LEU:HD23	4	0.13
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD21	4	0.13
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD22	4	0.13
(1,445)	1:45:A:LEU:HD22	1:80:A:LEU:HD23	4	0.13
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD21	4	0.13
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD22	4	0.13
(1,445)	1:45:A:LEU:HD23	1:80:A:LEU:HD23	4	0.13
(1,430)	1:43:A:ILE:HD11	1:128:A:ILE:HD11	1	0.13
(1,430)	1:43:A:ILE:HD11	1:128:A:ILE:HD12	1	0.13
(1,430)	1:43:A:ILE:HD11	1:128:A:ILE:HD13	1	0.13
(1,430)	1:43:A:ILE:HD12	1:128:A:ILE:HD11	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,430)	1:43:A:ILE:HD12	1:128:A:ILE:HD12	1	0.13
(1,430)	1:43:A:ILE:HD12	1:128:A:ILE:HD13	1	0.13
(1,430)	1:43:A:ILE:HD13	1:128:A:ILE:HD11	1	0.13
(1,430)	1:43:A:ILE:HD13	1:128:A:ILE:HD12	1	0.13
(1,430)	1:43:A:ILE:HD13	1:128:A:ILE:HD13	1	0.13
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	9	0.13
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	9	0.13
(1,429)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	9	0.13
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	9	0.13
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	9	0.13
(1,429)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	9	0.13
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	9	0.13
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	9	0.13
(1,429)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	9	0.13
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD21	10	0.13
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD22	10	0.13
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD23	10	0.13
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD21	10	0.13
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD22	10	0.13
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD23	10	0.13
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD21	10	0.13
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD22	10	0.13
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD23	10	0.13
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG11	6	0.13
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG12	6	0.13
(1,427)	1:33:A:ILE:HD11	1:136:A:VAL:HG13	6	0.13
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG11	6	0.13
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG12	6	0.13
(1,427)	1:33:A:ILE:HD12	1:136:A:VAL:HG13	6	0.13
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG11	6	0.13
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG12	6	0.13
(1,427)	1:33:A:ILE:HD13	1:136:A:VAL:HG13	6	0.13
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	6	0.13
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	6	0.13
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	6	0.13
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	6	0.13
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	6	0.13
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	6	0.13
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	6	0.13
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	6	0.13
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	6	0.13
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	6	0.13
(1,419)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	6	0.13
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	6	0.13
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	6	0.13
(1,419)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	6	0.13
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	6	0.13
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	6	0.13
(1,419)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	6	0.13
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	9	0.13
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	9	0.13
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	9	0.13
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	9	0.13
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	9	0.13
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	9	0.13
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	9	0.13
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	9	0.13
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	9	0.13
(1,403)	1:29:A:LEU:HD11	1:115:A:THR:HG21	3	0.13
(1,403)	1:29:A:LEU:HD11	1:115:A:THR:HG22	3	0.13
(1,403)	1:29:A:LEU:HD11	1:115:A:THR:HG23	3	0.13
(1,403)	1:29:A:LEU:HD12	1:115:A:THR:HG21	3	0.13
(1,403)	1:29:A:LEU:HD12	1:115:A:THR:HG22	3	0.13
(1,403)	1:29:A:LEU:HD12	1:115:A:THR:HG23	3	0.13
(1,403)	1:29:A:LEU:HD13	1:115:A:THR:HG21	3	0.13
(1,403)	1:29:A:LEU:HD13	1:115:A:THR:HG22	3	0.13
(1,403)	1:29:A:LEU:HD13	1:115:A:THR:HG23	3	0.13
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG21	8	0.13
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG22	8	0.13
(1,398)	1:26:A:ILE:HD11	1:115:A:THR:HG23	8	0.13
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG21	8	0.13
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG22	8	0.13
(1,398)	1:26:A:ILE:HD12	1:115:A:THR:HG23	8	0.13
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG21	8	0.13
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG22	8	0.13
(1,398)	1:26:A:ILE:HD13	1:115:A:THR:HG23	8	0.13
(1,347)	1:149:A:THR:H	1:187:A:ILE:H	10	0.13
(1,326)	1:81:A:ILE:H	1:90:A:THR:H	3	0.13
(1,313)	1:58:A:LYS:H	1:62:A:GLU:H	5	0.13
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	1	0.13
(1,286)	1:192:A:GLU:H	1:195:A:THR:H	2	0.13
(1,286)	1:192:A:GLU:H	1:195:A:THR:H	7	0.13
(1,279)	1:134:A:PHE:H	1:137:A:GLY:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:128:A:ILE:H	1:131:A:ILE:H	10	0.13
(1,162)	1:24:A:ALA:H	1:26:A:ILE:H	7	0.13
(1,133)	1:197:A:TYR:H	1:198:A:LEU:H	5	0.13
(1,119)	1:182:A:ARG:H	1:183:A:GLY:H	9	0.13
(1,77)	1:124:A:ALA:H	1:125:A:GLY:H	1	0.13
(1,69)	1:105:A:ASN:H	1:106:A:ASN:H	1	0.13
(1,69)	1:105:A:ASN:H	1:106:A:ASN:H	5	0.13
(1,41)	1:69:A:LYS:H	1:70:A:LEU:H	3	0.13
(2,100)	1:45:A:LEU:H	1:42:A:GLU:O	10	0.12
(2,98)	1:44:A:PHE:H	1:41:A:LYS:O	3	0.12
(2,70)	1:183:A:GLY:H	1:153:A:LYS:O	3	0.12
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	2	0.12
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	4	0.12
(2,32)	1:89:A:LEU:H	1:188:A:LEU:O	2	0.12
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG21	8	0.12
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG22	8	0.12
(1,1104)	1:231:A:SER:H	1:230:A:VAL:HG23	8	0.12
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG11	6	0.12
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG12	6	0.12
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG13	6	0.12
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG21	3	0.12
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG22	3	0.12
(1,1087)	1:220:A:LEU:H	1:219:A:THR:HG23	3	0.12
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD11	2	0.12
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD12	2	0.12
(1,1084)	1:216:A:TYR:H	1:218:A:ILE:HD13	2	0.12
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD21	4	0.12
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD22	4	0.12
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD23	4	0.12
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG21	1	0.12
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG22	1	0.12
(1,1077)	1:212:A:GLN:H	1:207:A:VAL:HG23	1	0.12
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG11	4	0.12
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG12	4	0.12
(1,1072)	1:209:A:LYS:H	1:207:A:VAL:HG13	4	0.12
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG11	3	0.12
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG12	3	0.12
(1,1057)	1:204:A:LYS:H	1:207:A:VAL:HG13	3	0.12
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD11	8	0.12
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD12	8	0.12
(1,1054)	1:204:A:LYS:H	1:45:A:LEU:HD13	8	0.12
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD11	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD12	5	0.12
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD13	5	0.12
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD21	5	0.12
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD22	5	0.12
(1,1048)	1:201:A:ARG:H	1:220:A:LEU:HD23	5	0.12
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD21	5	0.12
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD22	5	0.12
(1,1045)	1:200:A:GLU:H	1:220:A:LEU:HD23	5	0.12
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD21	4	0.12
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD22	4	0.12
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD23	4	0.12
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD11	1	0.12
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD12	1	0.12
(1,1032)	1:196:A:GLU:H	1:198:A:LEU:HD13	1	0.12
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB1	8	0.12
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB2	8	0.12
(1,1020)	1:190:A:LEU:H	1:145:A:ALA:HB3	8	0.12
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG21	8	0.12
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG22	8	0.12
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG23	8	0.12
(1,1012)	1:188:A:LEU:H	1:190:A:LEU:HD21	2	0.12
(1,1012)	1:188:A:LEU:H	1:190:A:LEU:HD22	2	0.12
(1,1012)	1:188:A:LEU:H	1:190:A:LEU:HD23	2	0.12
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	4	0.12
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	4	0.12
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	4	0.12
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG21	8	0.12
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG22	8	0.12
(1,967)	1:172:A:VAL:H	1:17:A:VAL:HG23	8	0.12
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG21	10	0.12
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG22	10	0.12
(1,957)	1:163:A:GLU:H	1:149:A:THR:HG23	10	0.12
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD11	10	0.12
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD12	10	0.12
(1,948)	1:162:A:TRP:H	1:103:A:LEU:HD13	10	0.12
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG21	2	0.12
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG22	2	0.12
(1,932)	1:151:A:ILE:H	1:149:A:THR:HG23	2	0.12
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB1	4	0.12
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB2	4	0.12
(1,919)	1:146:A:GLU:H	1:145:A:ALA:HB3	4	0.12
(1,916)	1:145:A:ALA:H	1:188:A:LEU:HD11	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:145:A:ALA:H	1:188:A:LEU:HD12	7	0.12
(1,916)	1:145:A:ALA:H	1:188:A:LEU:HD13	7	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD11	4	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD12	4	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD13	4	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD11	7	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD12	7	0.12
(1,893)	1:139:A:TYR:H	1:33:A:ILE:HD13	7	0.12
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG21	8	0.12
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG22	8	0.12
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG23	8	0.12
(1,884)	1:134:A:PHE:H	1:136:A:VAL:HG11	5	0.12
(1,884)	1:134:A:PHE:H	1:136:A:VAL:HG12	5	0.12
(1,884)	1:134:A:PHE:H	1:136:A:VAL:HG13	5	0.12
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE1	5	0.12
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE2	5	0.12
(1,882)	1:131:A:ILE:H	1:130:A:MET:HE3	5	0.12
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD11	7	0.12
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD12	7	0.12
(1,879)	1:128:A:ILE:H	1:122:A:LEU:HD13	7	0.12
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB1	10	0.12
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB2	10	0.12
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB3	10	0.12
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD11	7	0.12
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD12	7	0.12
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD13	7	0.12
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD21	5	0.12
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD22	5	0.12
(1,847)	1:104:A:ILE:H	1:103:A:LEU:HD23	5	0.12
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB1	4	0.12
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB2	4	0.12
(1,845)	1:104:A:ILE:H	1:101:A:ALA:HB3	4	0.12
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD11	6	0.12
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD12	6	0.12
(1,837)	1:95:A:GLY:H	1:56:A:LEU:HD13	6	0.12
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG21	9	0.12
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG22	9	0.12
(1,829)	1:92:A:VAL:H	1:90:A:THR:HG23	9	0.12
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD21	3	0.12
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD22	3	0.12
(1,815)	1:89:A:LEU:H	1:188:A:LEU:HD23	3	0.12
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD21	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD22	8	0.12
(1,802)	1:83:A:ASN:H	1:198:A:LEU:HD23	8	0.12
(1,751)	1:61:A:TYR:H	1:76:A:LEU:HD21	2	0.12
(1,751)	1:61:A:TYR:H	1:76:A:LEU:HD22	2	0.12
(1,751)	1:61:A:TYR:H	1:76:A:LEU:HD23	2	0.12
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG11	2	0.12
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG12	2	0.12
(1,716)	1:44:A:PHE:H	1:144:A:VAL:HG13	2	0.12
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	5	0.12
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	5	0.12
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	5	0.12
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB1	4	0.12
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB2	4	0.12
(1,695)	1:31:A:SER:H	1:166:A:ALA:HB3	4	0.12
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB1	5	0.12
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB2	5	0.12
(1,690)	1:29:A:LEU:H	1:27:A:ALA:HB3	5	0.12
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG11	9	0.12
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG12	9	0.12
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG13	9	0.12
(1,642)	1:144:A:VAL:H	1:144:A:VAL:HG11	1	0.12
(1,642)	1:144:A:VAL:H	1:144:A:VAL:HG12	1	0.12
(1,642)	1:144:A:VAL:H	1:144:A:VAL:HG13	1	0.12
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD11	2	0.12
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD12	2	0.12
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD13	2	0.12
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	6	0.12
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	6	0.12
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	6	0.12
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	6	0.12
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	6	0.12
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	6	0.12
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	6	0.12
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	6	0.12
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	6	0.12
(1,588)	1:203:A:ILE:HD11	1:220:A:LEU:HD11	3	0.12
(1,588)	1:203:A:ILE:HD11	1:220:A:LEU:HD12	3	0.12
(1,588)	1:203:A:ILE:HD11	1:220:A:LEU:HD13	3	0.12
(1,588)	1:203:A:ILE:HD12	1:220:A:LEU:HD11	3	0.12
(1,588)	1:203:A:ILE:HD12	1:220:A:LEU:HD12	3	0.12
(1,588)	1:203:A:ILE:HD12	1:220:A:LEU:HD13	3	0.12
(1,588)	1:203:A:ILE:HD13	1:220:A:LEU:HD11	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:203:A:ILE:HD13	1:220:A:LEU:HD12	3	0.12
(1,588)	1:203:A:ILE:HD13	1:220:A:LEU:HD13	3	0.12
(1,580)	1:188:A:LEU:HD11	1:190:A:LEU:HD21	2	0.12
(1,580)	1:188:A:LEU:HD11	1:190:A:LEU:HD22	2	0.12
(1,580)	1:188:A:LEU:HD11	1:190:A:LEU:HD23	2	0.12
(1,580)	1:188:A:LEU:HD12	1:190:A:LEU:HD21	2	0.12
(1,580)	1:188:A:LEU:HD12	1:190:A:LEU:HD22	2	0.12
(1,580)	1:188:A:LEU:HD12	1:190:A:LEU:HD23	2	0.12
(1,580)	1:188:A:LEU:HD13	1:190:A:LEU:HD21	2	0.12
(1,580)	1:188:A:LEU:HD13	1:190:A:LEU:HD22	2	0.12
(1,580)	1:188:A:LEU:HD13	1:190:A:LEU:HD23	2	0.12
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	4	0.12
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	4	0.12
(1,556)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	4	0.12
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	4	0.12
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	4	0.12
(1,556)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	4	0.12
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	4	0.12
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	4	0.12
(1,556)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	4	0.12
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	10	0.12
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	10	0.12
(1,551)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	10	0.12
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	10	0.12
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	10	0.12
(1,551)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	10	0.12
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	10	0.12
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	10	0.12
(1,551)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	10	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	5	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	5	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	5	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	5	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	5	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	5	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	5	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	5	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	5	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	10	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	10	0.12
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	10	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	10	0.12
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	10	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	10	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	10	0.12
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	10	0.12
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	2	0.12
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	2	0.12
(1,524)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	2	0.12
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	2	0.12
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	2	0.12
(1,524)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	2	0.12
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	2	0.12
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	2	0.12
(1,524)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	2	0.12
(1,523)	1:103:A:LEU:HD11	1:172:A:VAL:HG11	4	0.12
(1,523)	1:103:A:LEU:HD11	1:172:A:VAL:HG12	4	0.12
(1,523)	1:103:A:LEU:HD11	1:172:A:VAL:HG13	4	0.12
(1,523)	1:103:A:LEU:HD12	1:172:A:VAL:HG11	4	0.12
(1,523)	1:103:A:LEU:HD12	1:172:A:VAL:HG12	4	0.12
(1,523)	1:103:A:LEU:HD12	1:172:A:VAL:HG13	4	0.12
(1,523)	1:103:A:LEU:HD13	1:172:A:VAL:HG11	4	0.12
(1,523)	1:103:A:LEU:HD13	1:172:A:VAL:HG12	4	0.12
(1,523)	1:103:A:LEU:HD13	1:172:A:VAL:HG13	4	0.12
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG21	3	0.12
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG22	3	0.12
(1,522)	1:103:A:LEU:HD11	1:152:A:THR:HG23	3	0.12
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG21	3	0.12
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG22	3	0.12
(1,522)	1:103:A:LEU:HD12	1:152:A:THR:HG23	3	0.12
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG21	3	0.12
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG22	3	0.12
(1,522)	1:103:A:LEU:HD13	1:152:A:THR:HG23	3	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	5	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	5	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	5	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	5	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	5	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	5	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	5	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	5	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	5	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	9	0.12
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	9	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	9	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	9	0.12
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	9	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	9	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	9	0.12
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	9	0.12
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB1	9	0.12
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB2	9	0.12
(1,517)	1:99:A:THR:HG21	1:101:A:ALA:HB3	9	0.12
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB1	9	0.12
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB2	9	0.12
(1,517)	1:99:A:THR:HG22	1:101:A:ALA:HB3	9	0.12
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB1	9	0.12
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB2	9	0.12
(1,517)	1:99:A:THR:HG23	1:101:A:ALA:HB3	9	0.12
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG21	6	0.12
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG22	6	0.12
(1,514)	1:98:A:MET:HE1	1:150:A:VAL:HG23	6	0.12
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG21	6	0.12
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG22	6	0.12
(1,514)	1:98:A:MET:HE2	1:150:A:VAL:HG23	6	0.12
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG21	6	0.12
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG22	6	0.12
(1,514)	1:98:A:MET:HE3	1:150:A:VAL:HG23	6	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD11	8	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD12	8	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD13	8	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD11	8	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD12	8	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD13	8	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD11	8	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD12	8	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD13	8	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD11	9	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD12	9	0.12
(1,509)	1:98:A:MET:HE1	1:103:A:LEU:HD13	9	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD11	9	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD12	9	0.12
(1,509)	1:98:A:MET:HE2	1:103:A:LEU:HD13	9	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD11	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD12	9	0.12
(1,509)	1:98:A:MET:HE3	1:103:A:LEU:HD13	9	0.12
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE1	5	0.12
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE2	5	0.12
(1,508)	1:94:A:THR:HG21	1:180:A:MET:HE3	5	0.12
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE1	5	0.12
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE2	5	0.12
(1,508)	1:94:A:THR:HG22	1:180:A:MET:HE3	5	0.12
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE1	5	0.12
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE2	5	0.12
(1,508)	1:94:A:THR:HG23	1:180:A:MET:HE3	5	0.12
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	10	0.12
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	10	0.12
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	10	0.12
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	10	0.12
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	10	0.12
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	10	0.12
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	10	0.12
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	10	0.12
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	10	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	1	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	1	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	1	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	1	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	1	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	1	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	1	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	1	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	1	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	8	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	8	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	8	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	8	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	8	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	8	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	8	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	8	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	8	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	10	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	10	0.12
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	10	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	10	0.12
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	10	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	10	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	10	0.12
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	10	0.12
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	3	0.12
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	3	0.12
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	3	0.12
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	3	0.12
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	3	0.12
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	3	0.12
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	3	0.12
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	3	0.12
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	3	0.12
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	2	0.12
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	2	0.12
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	2	0.12
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	2	0.12
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	2	0.12
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	2	0.12
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	2	0.12
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	2	0.12
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	2	0.12
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	10	0.12
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	10	0.12
(1,493)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	10	0.12
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	10	0.12
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	10	0.12
(1,493)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	10	0.12
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	10	0.12
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	10	0.12
(1,493)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	10	0.12
(1,492)	1:89:A:LEU:HD11	1:203:A:ILE:HD11	4	0.12
(1,492)	1:89:A:LEU:HD11	1:203:A:ILE:HD12	4	0.12
(1,492)	1:89:A:LEU:HD11	1:203:A:ILE:HD13	4	0.12
(1,492)	1:89:A:LEU:HD12	1:203:A:ILE:HD11	4	0.12
(1,492)	1:89:A:LEU:HD12	1:203:A:ILE:HD12	4	0.12
(1,492)	1:89:A:LEU:HD12	1:203:A:ILE:HD13	4	0.12
(1,492)	1:89:A:LEU:HD13	1:203:A:ILE:HD11	4	0.12
(1,492)	1:89:A:LEU:HD13	1:203:A:ILE:HD12	4	0.12
(1,492)	1:89:A:LEU:HD13	1:203:A:ILE:HD13	4	0.12
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	8	0.12
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	8	0.12
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	8	0.12
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	8	0.12
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	8	0.12
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	8	0.12
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	8	0.12
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	8	0.12
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	9	0.12
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	9	0.12
(1,484)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	9	0.12
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	9	0.12
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	9	0.12
(1,484)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	9	0.12
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	9	0.12
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	9	0.12
(1,484)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	9	0.12
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	3	0.12
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	3	0.12
(1,482)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	3	0.12
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	3	0.12
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	3	0.12
(1,482)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	3	0.12
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	3	0.12
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	3	0.12
(1,482)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	3	0.12
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	8	0.12
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	8	0.12
(1,477)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	8	0.12
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	8	0.12
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	8	0.12
(1,477)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	8	0.12
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	8	0.12
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	8	0.12
(1,477)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	8	0.12
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	9	0.12
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	9	0.12
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	9	0.12
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	9	0.12
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	9	0.12
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	9	0.12
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	9	0.12
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	9	0.12
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	2	0.12
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	2	0.12
(1,463)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	2	0.12
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	2	0.12
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	2	0.12
(1,463)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	2	0.12
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	2	0.12
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	2	0.12
(1,463)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	2	0.12
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD11	5	0.12
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD12	5	0.12
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD13	5	0.12
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD11	5	0.12
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD12	5	0.12
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD13	5	0.12
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD11	5	0.12
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD12	5	0.12
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD13	5	0.12
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD11	10	0.12
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD12	10	0.12
(1,420)	1:32:A:LEU:HD11	1:128:A:ILE:HD13	10	0.12
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD11	10	0.12
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD12	10	0.12
(1,420)	1:32:A:LEU:HD12	1:128:A:ILE:HD13	10	0.12
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD11	10	0.12
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD12	10	0.12
(1,420)	1:32:A:LEU:HD13	1:128:A:ILE:HD13	10	0.12
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	8	0.12
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	8	0.12
(1,413)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	8	0.12
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	8	0.12
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	8	0.12
(1,413)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	8	0.12
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	8	0.12
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	8	0.12
(1,413)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	8	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG21	4	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG22	4	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG23	4	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG21	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG22	4	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG23	4	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG21	4	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG22	4	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG23	4	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG21	7	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG22	7	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG23	7	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG21	7	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG22	7	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG23	7	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG21	7	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG22	7	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG23	7	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG21	9	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG22	9	0.12
(1,411)	1:29:A:LEU:HD21	1:115:A:THR:HG23	9	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG21	9	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG22	9	0.12
(1,411)	1:29:A:LEU:HD22	1:115:A:THR:HG23	9	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG21	9	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG22	9	0.12
(1,411)	1:29:A:LEU:HD23	1:115:A:THR:HG23	9	0.12
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	4	0.12
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	4	0.12
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	4	0.12
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	4	0.12
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	4	0.12
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	4	0.12
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	4	0.12
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	4	0.12
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	4	0.12
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	9	0.12
(1,280)	1:136:A:VAL:H	1:139:A:TYR:H	10	0.12
(1,267)	1:99:A:THR:H	1:102:A:ASP:H	8	0.12
(1,243)	1:213:A:PHE:H	1:215:A:GLY:H	1	0.12
(1,227)	1:195:A:THR:H	1:197:A:TYR:H	1	0.12
(1,219)	1:164:A:SER:H	1:166:A:ALA:H	4	0.12
(1,218)	1:145:A:ALA:H	1:147:A:LYS:H	1	0.12
(1,208)	1:123:A:GLN:H	1:125:A:GLY:H	5	0.12
(1,151)	1:215:A:GLY:H	1:216:A:TYR:H	1	0.12
(1,110)	1:168:A:GLY:H	1:169:A:SER:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:117:A:ALA:H	1:118:A:PHE:H	2	0.12
(1,1)	1:36:A:THR:HG21	1:32:A:LEU:HD21	8	0.12
(1,1)	1:36:A:THR:HG21	1:32:A:LEU:HD22	8	0.12
(1,1)	1:36:A:THR:HG21	1:32:A:LEU:HD23	8	0.12
(1,1)	1:36:A:THR:HG22	1:32:A:LEU:HD21	8	0.12
(1,1)	1:36:A:THR:HG22	1:32:A:LEU:HD22	8	0.12
(1,1)	1:36:A:THR:HG22	1:32:A:LEU:HD23	8	0.12
(1,1)	1:36:A:THR:HG23	1:32:A:LEU:HD21	8	0.12
(1,1)	1:36:A:THR:HG23	1:32:A:LEU:HD22	8	0.12
(1,1)	1:36:A:THR:HG23	1:32:A:LEU:HD23	8	0.12
(2,148)	1:210:A:HIS:H	1:206:A:ILE:O	5	0.11
(2,128)	1:60:A:ARG:H	1:56:A:LEU:O	2	0.11
(2,86)	1:30:A:MET:H	1:26:A:ILE:O	4	0.11
(2,79)	1:190:A:LEU:N	1:87:A:ARG:O	7	0.11
(2,68)	1:153:A:LYS:H	1:183:A:GLY:O	5	0.11
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	10	0.11
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	3	0.11
(2,30)	1:88:A:THR:H	1:83:A:ASN:O	4	0.11
(2,16)	1:79:A:ASN:H	1:92:A:VAL:O	7	0.11
(2,2)	1:18:A:GLU:H	1:172:A:VAL:O	7	0.11
(1,1107)	1:123:A:GLN:HE21	1:32:A:LEU:HD21	7	0.11
(1,1107)	1:123:A:GLN:HE21	1:32:A:LEU:HD22	7	0.11
(1,1107)	1:123:A:GLN:HE21	1:32:A:LEU:HD23	7	0.11
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG11	3	0.11
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG12	3	0.11
(1,1103)	1:231:A:SER:H	1:230:A:VAL:HG13	3	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG11	3	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG12	3	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG13	3	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG11	8	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG12	8	0.11
(1,1100)	1:225:A:GLU:H	1:222:A:VAL:HG13	8	0.11
(1,1092)	1:221:A:PHE:H	1:220:A:LEU:HD11	7	0.11
(1,1092)	1:221:A:PHE:H	1:220:A:LEU:HD12	7	0.11
(1,1092)	1:221:A:PHE:H	1:220:A:LEU:HD13	7	0.11
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD21	9	0.11
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD22	9	0.11
(1,1081)	1:216:A:TYR:H	1:56:A:LEU:HD23	9	0.11
(1,1080)	1:214:A:ILE:H	1:218:A:ILE:HD11	8	0.11
(1,1080)	1:214:A:ILE:H	1:218:A:ILE:HD12	8	0.11
(1,1080)	1:214:A:ILE:H	1:218:A:ILE:HD13	8	0.11
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG21	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG22	1	0.11
(1,1075)	1:210:A:HIS:H	1:207:A:VAL:HG23	1	0.11
(1,1071)	1:208:A:LYS:H	1:207:A:VAL:HG21	1	0.11
(1,1071)	1:208:A:LYS:H	1:207:A:VAL:HG22	1	0.11
(1,1071)	1:208:A:LYS:H	1:207:A:VAL:HG23	1	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD11	1	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD12	1	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD13	1	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD11	2	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD12	2	0.11
(1,1058)	1:204:A:LYS:H	1:220:A:LEU:HD13	2	0.11
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD11	2	0.11
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD12	2	0.11
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD13	2	0.11
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD11	3	0.11
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD12	3	0.11
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD13	3	0.11
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD21	6	0.11
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD22	6	0.11
(1,1037)	1:197:A:TYR:H	1:198:A:LEU:HD23	6	0.11
(1,1027)	1:193:A:ASP:H	1:195:A:THR:HG21	9	0.11
(1,1027)	1:193:A:ASP:H	1:195:A:THR:HG22	9	0.11
(1,1027)	1:193:A:ASP:H	1:195:A:THR:HG23	9	0.11
(1,1011)	1:188:A:LEU:H	1:186:A:VAL:HG11	1	0.11
(1,1011)	1:188:A:LEU:H	1:186:A:VAL:HG12	1	0.11
(1,1011)	1:188:A:LEU:H	1:186:A:VAL:HG13	1	0.11
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG21	3	0.11
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG22	3	0.11
(1,1004)	1:188:A:LEU:H	1:88:A:THR:HG23	3	0.11
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD21	1	0.11
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD22	1	0.11
(1,1002)	1:187:A:ILE:H	1:188:A:LEU:HD23	1	0.11
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG11	5	0.11
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG12	5	0.11
(1,998)	1:187:A:ILE:H	1:150:A:VAL:HG13	5	0.11
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG21	2	0.11
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG22	2	0.11
(1,977)	1:177:A:GLY:H	1:176:A:THR:HG23	2	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB1	1	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB2	1	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB3	1	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB1	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB2	3	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB3	3	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB1	7	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB2	7	0.11
(1,974)	1:175:A:ASP:H	1:161:A:ALA:HB3	7	0.11
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD21	7	0.11
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD22	7	0.11
(1,970)	1:173:A:ARG:H	1:103:A:LEU:HD23	7	0.11
(1,963)	1:169:A:SER:H	1:30:A:MET:HE1	9	0.11
(1,963)	1:169:A:SER:H	1:30:A:MET:HE2	9	0.11
(1,963)	1:169:A:SER:H	1:30:A:MET:HE3	9	0.11
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	8	0.11
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	8	0.11
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	8	0.11
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	9	0.11
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	9	0.11
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	9	0.11
(1,943)	1:160:A:TYR:H	1:103:A:LEU:HD21	10	0.11
(1,943)	1:160:A:TYR:H	1:103:A:LEU:HD22	10	0.11
(1,943)	1:160:A:TYR:H	1:103:A:LEU:HD23	10	0.11
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE1	3	0.11
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE2	3	0.11
(1,941)	1:153:A:LYS:H	1:180:A:MET:HE3	3	0.11
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG21	8	0.11
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG22	8	0.11
(1,940)	1:153:A:LYS:H	1:152:A:THR:HG23	8	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE1	8	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE2	8	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE3	8	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE1	10	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE2	10	0.11
(1,930)	1:151:A:ILE:H	1:98:A:MET:HE3	10	0.11
(1,912)	1:144:A:VAL:H	1:190:A:LEU:HD21	9	0.11
(1,912)	1:144:A:VAL:H	1:190:A:LEU:HD22	9	0.11
(1,912)	1:144:A:VAL:H	1:190:A:LEU:HD23	9	0.11
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD11	1	0.11
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD12	1	0.11
(1,898)	1:141:A:ALA:H	1:131:A:ILE:HD13	1	0.11
(1,894)	1:139:A:TYR:H	1:48:A:LEU:HD11	8	0.11
(1,894)	1:139:A:TYR:H	1:48:A:LEU:HD12	8	0.11
(1,894)	1:139:A:TYR:H	1:48:A:LEU:HD13	8	0.11
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG21	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG22	4	0.11
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG23	4	0.11
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG21	7	0.11
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG22	7	0.11
(1,891)	1:138:A:PHE:H	1:136:A:VAL:HG23	7	0.11
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG21	2	0.11
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG22	2	0.11
(1,889)	1:138:A:PHE:H	1:109:A:THR:HG23	2	0.11
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD11	6	0.11
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD12	6	0.11
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD13	6	0.11
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD11	8	0.11
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD12	8	0.11
(1,888)	1:138:A:PHE:H	1:48:A:LEU:HD13	8	0.11
(1,883)	1:133:A:GLN:H	1:136:A:VAL:HG11	8	0.11
(1,883)	1:133:A:GLN:H	1:136:A:VAL:HG12	8	0.11
(1,883)	1:133:A:GLN:H	1:136:A:VAL:HG13	8	0.11
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB1	10	0.11
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB2	10	0.11
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB3	10	0.11
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB1	10	0.11
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB2	10	0.11
(1,863)	1:122:A:LEU:H	1:126:A:ALA:HB3	10	0.11
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB1	6	0.11
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB2	6	0.11
(1,862)	1:122:A:LEU:H	1:124:A:ALA:HB3	6	0.11
(1,858)	1:118:A:PHE:H	1:136:A:VAL:HG11	7	0.11
(1,858)	1:118:A:PHE:H	1:136:A:VAL:HG12	7	0.11
(1,858)	1:118:A:PHE:H	1:136:A:VAL:HG13	7	0.11
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG21	9	0.11
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG22	9	0.11
(1,855)	1:118:A:PHE:H	1:115:A:THR:HG23	9	0.11
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD11	9	0.11
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD12	9	0.11
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD13	9	0.11
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD11	10	0.11
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD12	10	0.11
(1,850)	1:105:A:ASN:H	1:104:A:ILE:HD13	10	0.11
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD11	2	0.11
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD12	2	0.11
(1,846)	1:104:A:ILE:H	1:103:A:LEU:HD13	2	0.11
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD11	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD12	10	0.11
(1,836)	1:94:A:THR:H	1:56:A:LEU:HD13	10	0.11
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG21	1	0.11
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG22	1	0.11
(1,835)	1:93:A:ASP:H	1:184:A:THR:HG23	1	0.11
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD21	6	0.11
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD22	6	0.11
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD23	6	0.11
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG11	2	0.11
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG12	2	0.11
(1,784)	1:79:A:ASN:H	1:92:A:VAL:HG13	2	0.11
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG21	6	0.11
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG22	6	0.11
(1,779)	1:78:A:ILE:H	1:94:A:THR:HG23	6	0.11
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD21	6	0.11
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD22	6	0.11
(1,757)	1:63:A:SER:H	1:70:A:LEU:HD23	6	0.11
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD11	4	0.11
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD12	4	0.11
(1,749)	1:61:A:TYR:H	1:64:A:LEU:HD13	4	0.11
(1,738)	1:57:A:ASP:H	1:56:A:LEU:HD21	8	0.11
(1,738)	1:57:A:ASP:H	1:56:A:LEU:HD22	8	0.11
(1,738)	1:57:A:ASP:H	1:56:A:LEU:HD23	8	0.11
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB1	5	0.11
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB2	5	0.11
(1,735)	1:56:A:LEU:H	1:55:A:ALA:HB3	5	0.11
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	9	0.11
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	9	0.11
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	9	0.11
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD11	10	0.11
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD12	10	0.11
(1,706)	1:35:A:ASN:H	1:32:A:LEU:HD13	10	0.11
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	10	0.11
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	10	0.11
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	10	0.11
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG21	10	0.11
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG22	10	0.11
(1,685)	1:26:A:ILE:H	1:115:A:THR:HG23	10	0.11
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG21	9	0.11
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG22	9	0.11
(1,675)	1:18:A:GLU:H	1:172:A:VAL:HG23	9	0.11
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG11	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG12	7	0.11
(1,674)	1:18:A:GLU:H	1:172:A:VAL:HG13	7	0.11
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG11	3	0.11
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG12	3	0.11
(1,649)	1:172:A:VAL:H	1:172:A:VAL:HG13	3	0.11
(1,630)	1:103:A:LEU:H	1:103:A:LEU:HD21	3	0.11
(1,630)	1:103:A:LEU:H	1:103:A:LEU:HD22	3	0.11
(1,630)	1:103:A:LEU:H	1:103:A:LEU:HD23	3	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD11	1	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD12	1	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD13	1	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD11	9	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD12	9	0.11
(1,625)	1:91:A:ILE:H	1:91:A:ILE:HD13	9	0.11
(1,621)	1:80:A:LEU:H	1:80:A:LEU:HD21	10	0.11
(1,621)	1:80:A:LEU:H	1:80:A:LEU:HD22	10	0.11
(1,621)	1:80:A:LEU:H	1:80:A:LEU:HD23	10	0.11
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD11	8	0.11
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD12	8	0.11
(1,612)	1:59:A:ILE:H	1:59:A:ILE:HD13	8	0.11
(1,583)	1:190:A:LEU:HD11	1:198:A:LEU:HD21	7	0.11
(1,583)	1:190:A:LEU:HD11	1:198:A:LEU:HD22	7	0.11
(1,583)	1:190:A:LEU:HD11	1:198:A:LEU:HD23	7	0.11
(1,583)	1:190:A:LEU:HD12	1:198:A:LEU:HD21	7	0.11
(1,583)	1:190:A:LEU:HD12	1:198:A:LEU:HD22	7	0.11
(1,583)	1:190:A:LEU:HD12	1:198:A:LEU:HD23	7	0.11
(1,583)	1:190:A:LEU:HD13	1:198:A:LEU:HD21	7	0.11
(1,583)	1:190:A:LEU:HD13	1:198:A:LEU:HD22	7	0.11
(1,583)	1:190:A:LEU:HD13	1:198:A:LEU:HD23	7	0.11
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	2	0.11
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	2	0.11
(1,578)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	2	0.11
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	2	0.11
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	2	0.11
(1,578)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	2	0.11
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	2	0.11
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	2	0.11
(1,578)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	2	0.11
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG21	6	0.11
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG22	6	0.11
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG23	6	0.11
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG21	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG22	6	0.11
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG23	6	0.11
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG21	6	0.11
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG22	6	0.11
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG23	6	0.11
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	9	0.11
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	9	0.11
(1,553)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	9	0.11
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	9	0.11
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	9	0.11
(1,553)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	9	0.11
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	9	0.11
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	9	0.11
(1,553)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	9	0.11
(1,538)	1:115:A:THR:HG21	1:136:A:VAL:HG21	6	0.11
(1,538)	1:115:A:THR:HG21	1:136:A:VAL:HG22	6	0.11
(1,538)	1:115:A:THR:HG21	1:136:A:VAL:HG23	6	0.11
(1,538)	1:115:A:THR:HG22	1:136:A:VAL:HG21	6	0.11
(1,538)	1:115:A:THR:HG22	1:136:A:VAL:HG22	6	0.11
(1,538)	1:115:A:THR:HG22	1:136:A:VAL:HG23	6	0.11
(1,538)	1:115:A:THR:HG23	1:136:A:VAL:HG21	6	0.11
(1,538)	1:115:A:THR:HG23	1:136:A:VAL:HG22	6	0.11
(1,538)	1:115:A:THR:HG23	1:136:A:VAL:HG23	6	0.11
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	1	0.11
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	1	0.11
(1,519)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	1	0.11
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	1	0.11
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	1	0.11
(1,519)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	1	0.11
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	1	0.11
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	1	0.11
(1,519)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	1	0.11
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD21	1	0.11
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD22	1	0.11
(1,510)	1:98:A:MET:HE1	1:103:A:LEU:HD23	1	0.11
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD21	1	0.11
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD22	1	0.11
(1,510)	1:98:A:MET:HE2	1:103:A:LEU:HD23	1	0.11
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD21	1	0.11
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD22	1	0.11
(1,510)	1:98:A:MET:HE3	1:103:A:LEU:HD23	1	0.11
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD11	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD12	2	0.11
(1,500)	1:90:A:THR:HG21	1:187:A:ILE:HD13	2	0.11
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD11	2	0.11
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD12	2	0.11
(1,500)	1:90:A:THR:HG22	1:187:A:ILE:HD13	2	0.11
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD11	2	0.11
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD12	2	0.11
(1,500)	1:90:A:THR:HG23	1:187:A:ILE:HD13	2	0.11
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	4	0.11
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	4	0.11
(1,495)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	4	0.11
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	4	0.11
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	4	0.11
(1,495)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	4	0.11
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	4	0.11
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	4	0.11
(1,495)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	4	0.11
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD11	3	0.11
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD12	3	0.11
(1,490)	1:89:A:LEU:HD11	1:91:A:ILE:HD13	3	0.11
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD11	3	0.11
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD12	3	0.11
(1,490)	1:89:A:LEU:HD12	1:91:A:ILE:HD13	3	0.11
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD11	3	0.11
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD12	3	0.11
(1,490)	1:89:A:LEU:HD13	1:91:A:ILE:HD13	3	0.11
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	2	0.11
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	2	0.11
(1,476)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	2	0.11
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	2	0.11
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	2	0.11
(1,476)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	2	0.11
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	2	0.11
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	2	0.11
(1,476)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	2	0.11
(1,475)	1:64:A:LEU:HD11	1:65:A:THR:HG21	6	0.11
(1,475)	1:64:A:LEU:HD11	1:65:A:THR:HG22	6	0.11
(1,475)	1:64:A:LEU:HD11	1:65:A:THR:HG23	6	0.11
(1,475)	1:64:A:LEU:HD12	1:65:A:THR:HG21	6	0.11
(1,475)	1:64:A:LEU:HD12	1:65:A:THR:HG22	6	0.11
(1,475)	1:64:A:LEU:HD12	1:65:A:THR:HG23	6	0.11
(1,475)	1:64:A:LEU:HD13	1:65:A:THR:HG21	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:64:A:LEU:HD13	1:65:A:THR:HG22	6	0.11
(1,475)	1:64:A:LEU:HD13	1:65:A:THR:HG23	6	0.11
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	1	0.11
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	1	0.11
(1,464)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	1	0.11
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	1	0.11
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	1	0.11
(1,464)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	1	0.11
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	1	0.11
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	1	0.11
(1,464)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	1	0.11
(1,461)	1:49:A:ILE:HD11	1:80:A:LEU:HD11	8	0.11
(1,461)	1:49:A:ILE:HD11	1:80:A:LEU:HD12	8	0.11
(1,461)	1:49:A:ILE:HD11	1:80:A:LEU:HD13	8	0.11
(1,461)	1:49:A:ILE:HD12	1:80:A:LEU:HD11	8	0.11
(1,461)	1:49:A:ILE:HD12	1:80:A:LEU:HD12	8	0.11
(1,461)	1:49:A:ILE:HD12	1:80:A:LEU:HD13	8	0.11
(1,461)	1:49:A:ILE:HD13	1:80:A:LEU:HD11	8	0.11
(1,461)	1:49:A:ILE:HD13	1:80:A:LEU:HD12	8	0.11
(1,461)	1:49:A:ILE:HD13	1:80:A:LEU:HD13	8	0.11
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	7	0.11
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	7	0.11
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	7	0.11
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	7	0.11
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	7	0.11
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	7	0.11
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	7	0.11
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	7	0.11
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	7	0.11
(1,436)	1:45:A:LEU:HD11	1:89:A:LEU:HD11	10	0.11
(1,436)	1:45:A:LEU:HD11	1:89:A:LEU:HD12	10	0.11
(1,436)	1:45:A:LEU:HD11	1:89:A:LEU:HD13	10	0.11
(1,436)	1:45:A:LEU:HD12	1:89:A:LEU:HD11	10	0.11
(1,436)	1:45:A:LEU:HD12	1:89:A:LEU:HD12	10	0.11
(1,436)	1:45:A:LEU:HD12	1:89:A:LEU:HD13	10	0.11
(1,436)	1:45:A:LEU:HD13	1:89:A:LEU:HD11	10	0.11
(1,436)	1:45:A:LEU:HD13	1:89:A:LEU:HD12	10	0.11
(1,436)	1:45:A:LEU:HD13	1:89:A:LEU:HD13	10	0.11
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	2	0.11
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	2	0.11
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	2	0.11
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	2	0.11
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	2	0.11
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	2	0.11
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	2	0.11
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	2	0.11
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	8	0.11
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	8	0.11
(1,423)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	8	0.11
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	8	0.11
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	8	0.11
(1,423)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	8	0.11
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	8	0.11
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	8	0.11
(1,423)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	8	0.11
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	1	0.11
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	1	0.11
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	1	0.11
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	1	0.11
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	1	0.11
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	1	0.11
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	1	0.11
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	1	0.11
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	1	0.11
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	9	0.11
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	9	0.11
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	9	0.11
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	9	0.11
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	9	0.11
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	9	0.11
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	9	0.11
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	9	0.11
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	9	0.11
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	1	0.11
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	1	0.11
(1,399)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	1	0.11
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	1	0.11
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	1	0.11
(1,399)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	1	0.11
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	1	0.11
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	1	0.11
(1,399)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	1	0.11
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	8	0.11
(1,396)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	8	0.11
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	8	0.11
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	8	0.11
(1,396)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	8	0.11
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	8	0.11
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	8	0.11
(1,396)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	8	0.11
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG21	9	0.11
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG22	9	0.11
(1,395)	1:19:A:THR:HG21	1:171:A:THR:HG23	9	0.11
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG21	9	0.11
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG22	9	0.11
(1,395)	1:19:A:THR:HG22	1:171:A:THR:HG23	9	0.11
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG21	9	0.11
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG22	9	0.11
(1,395)	1:19:A:THR:HG23	1:171:A:THR:HG23	9	0.11
(1,364)	1:225:A:GLU:H	1:230:A:VAL:H	2	0.11
(1,349)	1:150:A:VAL:H	1:162:A:TRP:H	4	0.11
(1,342)	1:146:A:GLU:H	1:191:A:LYS:H	6	0.11
(1,337)	1:103:A:LEU:H	1:107:A:LEU:H	6	0.11
(1,314)	1:58:A:LYS:H	1:96:A:ILE:H	4	0.11
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	7	0.11
(1,277)	1:131:A:ILE:H	1:134:A:PHE:H	10	0.11
(1,218)	1:145:A:ALA:H	1:147:A:LYS:H	5	0.11
(1,16)	1:38:A:TYR:H	1:39:A:SER:H	10	0.11
(2,97)	1:44:A:PHE:N	1:41:A:LYS:O	2	0.1
(2,97)	1:44:A:PHE:N	1:41:A:LYS:O	3	0.1
(2,92)	1:33:A:ILE:H	1:29:A:LEU:O	9	0.1
(2,82)	1:28:A:GLN:H	1:24:A:ALA:O	1	0.1
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	7	0.1
(2,42)	1:184:A:THR:H	1:93:A:ASP:O	5	0.1
(1,1105)	1:123:A:GLN:HE21	1:119:A:MET:HE1	6	0.1
(1,1105)	1:123:A:GLN:HE21	1:119:A:MET:HE2	6	0.1
(1,1105)	1:123:A:GLN:HE21	1:119:A:MET:HE3	6	0.1
(1,1102)	1:226:A:ARG:H	1:230:A:VAL:HG11	5	0.1
(1,1102)	1:226:A:ARG:H	1:230:A:VAL:HG12	5	0.1
(1,1102)	1:226:A:ARG:H	1:230:A:VAL:HG13	5	0.1
(1,1070)	1:208:A:LYS:H	1:207:A:VAL:HG11	8	0.1
(1,1070)	1:208:A:LYS:H	1:207:A:VAL:HG12	8	0.1
(1,1070)	1:208:A:LYS:H	1:207:A:VAL:HG13	8	0.1
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD11	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD12	1	0.1
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD13	1	0.1
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD11	8	0.1
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD12	8	0.1
(1,1051)	1:203:A:ILE:H	1:206:A:ILE:HD13	8	0.1
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG21	5	0.1
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG22	5	0.1
(1,1013)	1:189:A:HIS:H	1:88:A:THR:HG23	5	0.1
(1,984)	1:185:A:LYS:H	1:150:A:VAL:HG11	1	0.1
(1,984)	1:185:A:LYS:H	1:150:A:VAL:HG12	1	0.1
(1,984)	1:185:A:LYS:H	1:150:A:VAL:HG13	1	0.1
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG21	4	0.1
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG22	4	0.1
(1,965)	1:170:A:PHE:H	1:19:A:THR:HG23	4	0.1
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG11	2	0.1
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG12	2	0.1
(1,961)	1:164:A:SER:H	1:148:A:VAL:HG13	2	0.1
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB1	1	0.1
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB2	1	0.1
(1,954)	1:162:A:TRP:H	1:161:A:ALA:HB3	1	0.1
(1,953)	1:162:A:TRP:H	1:151:A:ILE:HD11	3	0.1
(1,953)	1:162:A:TRP:H	1:151:A:ILE:HD12	3	0.1
(1,953)	1:162:A:TRP:H	1:151:A:ILE:HD13	3	0.1
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG21	7	0.1
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG22	7	0.1
(1,928)	1:150:A:VAL:H	1:149:A:THR:HG23	7	0.1
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD21	1	0.1
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD22	1	0.1
(1,921)	1:146:A:GLU:H	1:190:A:LEU:HD23	1	0.1
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG21	6	0.1
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG22	6	0.1
(1,909)	1:143:A:LEU:H	1:144:A:VAL:HG23	6	0.1
(1,874)	1:126:A:ALA:H	1:130:A:MET:HE1	3	0.1
(1,874)	1:126:A:ALA:H	1:130:A:MET:HE2	3	0.1
(1,874)	1:126:A:ALA:H	1:130:A:MET:HE3	3	0.1
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB1	9	0.1
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB2	9	0.1
(1,870)	1:125:A:GLY:H	1:124:A:ALA:HB3	9	0.1
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB1	4	0.1
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB2	4	0.1
(1,868)	1:123:A:GLN:H	1:126:A:ALA:HB3	4	0.1
(1,840)	1:96:A:ILE:H	1:55:A:ALA:HB1	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:96:A:ILE:H	1:55:A:ALA:HB2	5	0.1
(1,840)	1:96:A:ILE:H	1:55:A:ALA:HB3	5	0.1
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD21	8	0.1
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD22	8	0.1
(1,827)	1:92:A:VAL:H	1:80:A:LEU:HD23	8	0.1
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD21	2	0.1
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD22	2	0.1
(1,812)	1:87:A:ARG:H	1:198:A:LEU:HD23	2	0.1
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG21	6	0.1
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG22	6	0.1
(1,810)	1:87:A:ARG:H	1:88:A:THR:HG23	6	0.1
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD11	5	0.1
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD12	5	0.1
(1,797)	1:81:A:ILE:H	1:220:A:LEU:HD13	5	0.1
(1,788)	1:80:A:LEU:H	1:220:A:LEU:HD11	10	0.1
(1,788)	1:80:A:LEU:H	1:220:A:LEU:HD12	10	0.1
(1,788)	1:80:A:LEU:H	1:220:A:LEU:HD13	10	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD21	2	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD22	2	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD23	2	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD21	9	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD22	9	0.1
(1,781)	1:79:A:ASN:H	1:80:A:LEU:HD23	9	0.1
(1,766)	1:71:A:ASP:H	1:70:A:LEU:HD21	5	0.1
(1,766)	1:71:A:ASP:H	1:70:A:LEU:HD22	5	0.1
(1,766)	1:71:A:ASP:H	1:70:A:LEU:HD23	5	0.1
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD11	6	0.1
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD12	6	0.1
(1,765)	1:71:A:ASP:H	1:70:A:LEU:HD13	6	0.1
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD11	1	0.1
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD12	1	0.1
(1,737)	1:57:A:ASP:H	1:56:A:LEU:HD13	1	0.1
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD11	2	0.1
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD12	2	0.1
(1,705)	1:34:A:ILE:H	1:33:A:ILE:HD13	2	0.1
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD21	1	0.1
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD22	1	0.1
(1,701)	1:33:A:ILE:H	1:32:A:LEU:HD23	1	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB1	1	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB2	1	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB3	1	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB1	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB2	5	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB3	5	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB1	6	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB2	6	0.1
(1,689)	1:28:A:GLN:H	1:27:A:ALA:HB3	6	0.1
(1,679)	1:21:A:ALA:H	1:19:A:THR:HG21	6	0.1
(1,679)	1:21:A:ALA:H	1:19:A:THR:HG22	6	0.1
(1,679)	1:21:A:ALA:H	1:19:A:THR:HG23	6	0.1
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD11	7	0.1
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD12	7	0.1
(1,656)	1:190:A:LEU:H	1:190:A:LEU:HD13	7	0.1
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD21	5	0.1
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD22	5	0.1
(1,633)	1:107:A:LEU:H	1:107:A:LEU:HD23	5	0.1
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	8	0.1
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	8	0.1
(1,596)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	8	0.1
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	8	0.1
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	8	0.1
(1,596)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	8	0.1
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	8	0.1
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	8	0.1
(1,596)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	8	0.1
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD21	7	0.1
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD22	7	0.1
(1,581)	1:188:A:LEU:HD21	1:190:A:LEU:HD23	7	0.1
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD21	7	0.1
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD22	7	0.1
(1,581)	1:188:A:LEU:HD22	1:190:A:LEU:HD23	7	0.1
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD21	7	0.1
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD22	7	0.1
(1,581)	1:188:A:LEU:HD23	1:190:A:LEU:HD23	7	0.1
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG21	1	0.1
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG22	1	0.1
(1,569)	1:150:A:VAL:HG21	1:152:A:THR:HG23	1	0.1
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG21	1	0.1
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG22	1	0.1
(1,569)	1:150:A:VAL:HG22	1:152:A:THR:HG23	1	0.1
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG21	1	0.1
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG22	1	0.1
(1,569)	1:150:A:VAL:HG23	1:152:A:THR:HG23	1	0.1
(1,561)	1:148:A:VAL:HG11	1:188:A:LEU:HD21	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:148:A:VAL:HG11	1:188:A:LEU:HD22	2	0.1
(1,561)	1:148:A:VAL:HG11	1:188:A:LEU:HD23	2	0.1
(1,561)	1:148:A:VAL:HG12	1:188:A:LEU:HD21	2	0.1
(1,561)	1:148:A:VAL:HG12	1:188:A:LEU:HD22	2	0.1
(1,561)	1:148:A:VAL:HG12	1:188:A:LEU:HD23	2	0.1
(1,561)	1:148:A:VAL:HG13	1:188:A:LEU:HD21	2	0.1
(1,561)	1:148:A:VAL:HG13	1:188:A:LEU:HD22	2	0.1
(1,561)	1:148:A:VAL:HG13	1:188:A:LEU:HD23	2	0.1
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	8	0.1
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	8	0.1
(1,540)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	8	0.1
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	8	0.1
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	8	0.1
(1,540)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	8	0.1
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	8	0.1
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	8	0.1
(1,540)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	8	0.1
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD21	5	0.1
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD22	5	0.1
(1,539)	1:119:A:MET:HE1	1:122:A:LEU:HD23	5	0.1
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD21	5	0.1
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD22	5	0.1
(1,539)	1:119:A:MET:HE2	1:122:A:LEU:HD23	5	0.1
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD21	5	0.1
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD22	5	0.1
(1,539)	1:119:A:MET:HE3	1:122:A:LEU:HD23	5	0.1
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	5	0.1
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	5	0.1
(1,502)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	5	0.1
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	5	0.1
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	5	0.1
(1,502)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	5	0.1
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	5	0.1
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	5	0.1
(1,502)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	5	0.1
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	2	0.1
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	2	0.1
(1,497)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	2	0.1
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	2	0.1
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	2	0.1
(1,497)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	2	0.1
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	2	0.1
(1,497)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	2	0.1
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD11	1	0.1
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD12	1	0.1
(1,479)	1:78:A:ILE:HD11	1:218:A:ILE:HD13	1	0.1
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD11	1	0.1
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD12	1	0.1
(1,479)	1:78:A:ILE:HD12	1:218:A:ILE:HD13	1	0.1
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD11	1	0.1
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD12	1	0.1
(1,479)	1:78:A:ILE:HD13	1:218:A:ILE:HD13	1	0.1
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	4	0.1
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	4	0.1
(1,470)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	4	0.1
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	4	0.1
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	4	0.1
(1,470)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	4	0.1
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	4	0.1
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	4	0.1
(1,470)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	4	0.1
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD11	2	0.1
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD12	2	0.1
(1,455)	1:48:A:LEU:HD21	1:91:A:ILE:HD13	2	0.1
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD11	2	0.1
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD12	2	0.1
(1,455)	1:48:A:LEU:HD22	1:91:A:ILE:HD13	2	0.1
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD11	2	0.1
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD12	2	0.1
(1,455)	1:48:A:LEU:HD23	1:91:A:ILE:HD13	2	0.1
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD11	6	0.1
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD12	6	0.1
(1,443)	1:45:A:LEU:HD21	1:49:A:ILE:HD13	6	0.1
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD11	6	0.1
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD12	6	0.1
(1,443)	1:45:A:LEU:HD22	1:49:A:ILE:HD13	6	0.1
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD11	6	0.1
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD12	6	0.1
(1,443)	1:45:A:LEU:HD23	1:49:A:ILE:HD13	6	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD11	6	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD12	6	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD13	6	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD11	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD12	6	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD13	6	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD11	6	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD12	6	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD13	6	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD11	8	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD12	8	0.1
(1,434)	1:45:A:LEU:HD11	1:80:A:LEU:HD13	8	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD11	8	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD12	8	0.1
(1,434)	1:45:A:LEU:HD12	1:80:A:LEU:HD13	8	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD11	8	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD12	8	0.1
(1,434)	1:45:A:LEU:HD13	1:80:A:LEU:HD13	8	0.1
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD21	3	0.1
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD22	3	0.1
(1,428)	1:33:A:ILE:HD11	1:143:A:LEU:HD23	3	0.1
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD21	3	0.1
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD22	3	0.1
(1,428)	1:33:A:ILE:HD12	1:143:A:LEU:HD23	3	0.1
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD21	3	0.1
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD22	3	0.1
(1,428)	1:33:A:ILE:HD13	1:143:A:LEU:HD23	3	0.1
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD11	2	0.1
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD12	2	0.1
(1,425)	1:32:A:LEU:HD21	1:128:A:ILE:HD13	2	0.1
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD11	2	0.1
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD12	2	0.1
(1,425)	1:32:A:LEU:HD22	1:128:A:ILE:HD13	2	0.1
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD11	2	0.1
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD12	2	0.1
(1,425)	1:32:A:LEU:HD23	1:128:A:ILE:HD13	2	0.1
(1,424)	1:32:A:LEU:HD21	1:122:A:LEU:HD21	5	0.1
(1,424)	1:32:A:LEU:HD21	1:122:A:LEU:HD22	5	0.1
(1,424)	1:32:A:LEU:HD21	1:122:A:LEU:HD23	5	0.1
(1,424)	1:32:A:LEU:HD22	1:122:A:LEU:HD21	5	0.1
(1,424)	1:32:A:LEU:HD22	1:122:A:LEU:HD22	5	0.1
(1,424)	1:32:A:LEU:HD22	1:122:A:LEU:HD23	5	0.1
(1,424)	1:32:A:LEU:HD23	1:122:A:LEU:HD21	5	0.1
(1,424)	1:32:A:LEU:HD23	1:122:A:LEU:HD22	5	0.1
(1,424)	1:32:A:LEU:HD23	1:122:A:LEU:HD23	5	0.1
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	6	0.1
(1,401)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	6	0.1
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	6	0.1
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	6	0.1
(1,401)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	6	0.1
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	6	0.1
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	6	0.1
(1,401)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	6	0.1
(1,394)	1:17:A:VAL:HG11	1:171:A:THR:HG21	6	0.1
(1,394)	1:17:A:VAL:HG11	1:171:A:THR:HG22	6	0.1
(1,394)	1:17:A:VAL:HG11	1:171:A:THR:HG23	6	0.1
(1,394)	1:17:A:VAL:HG12	1:171:A:THR:HG21	6	0.1
(1,394)	1:17:A:VAL:HG12	1:171:A:THR:HG22	6	0.1
(1,394)	1:17:A:VAL:HG12	1:171:A:THR:HG23	6	0.1
(1,394)	1:17:A:VAL:HG13	1:171:A:THR:HG21	6	0.1
(1,394)	1:17:A:VAL:HG13	1:171:A:THR:HG22	6	0.1
(1,394)	1:17:A:VAL:HG13	1:171:A:THR:HG23	6	0.1
(1,352)	1:152:A:THR:H	1:160:A:TYR:H	3	0.1
(1,346)	1:148:A:VAL:H	1:164:A:SER:H	9	0.1
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	4	0.1
(1,221)	1:180:A:MET:H	1:182:A:ARG:H	2	0.1
(1,220)	1:167:A:GLY:H	1:169:A:SER:H	7	0.1
(1,151)	1:215:A:GLY:H	1:216:A:TYR:H	6	0.1
(1,151)	1:215:A:GLY:H	1:216:A:TYR:H	7	0.1
(1,81)	1:128:A:ILE:H	1:129:A:SER:H	2	0.1
(1,78)	1:125:A:GLY:H	1:126:A:ALA:H	6	0.1
(1,16)	1:38:A:TYR:H	1:39:A:SER:H	6	0.1

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

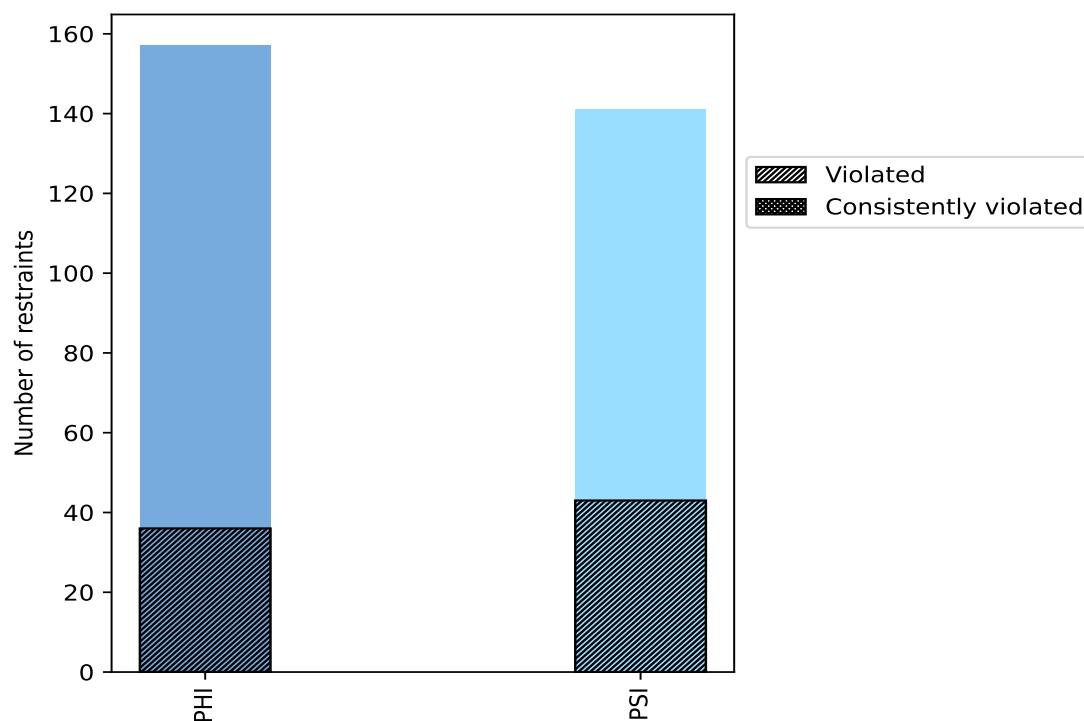
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	157	52.7	36	22.9	12.1	0	0.0	0.0
PSI	141	47.3	43	30.5	14.4	0	0.0	0.0
Total	298	100.0	79	26.5	26.5	0	0.0	0.0

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

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



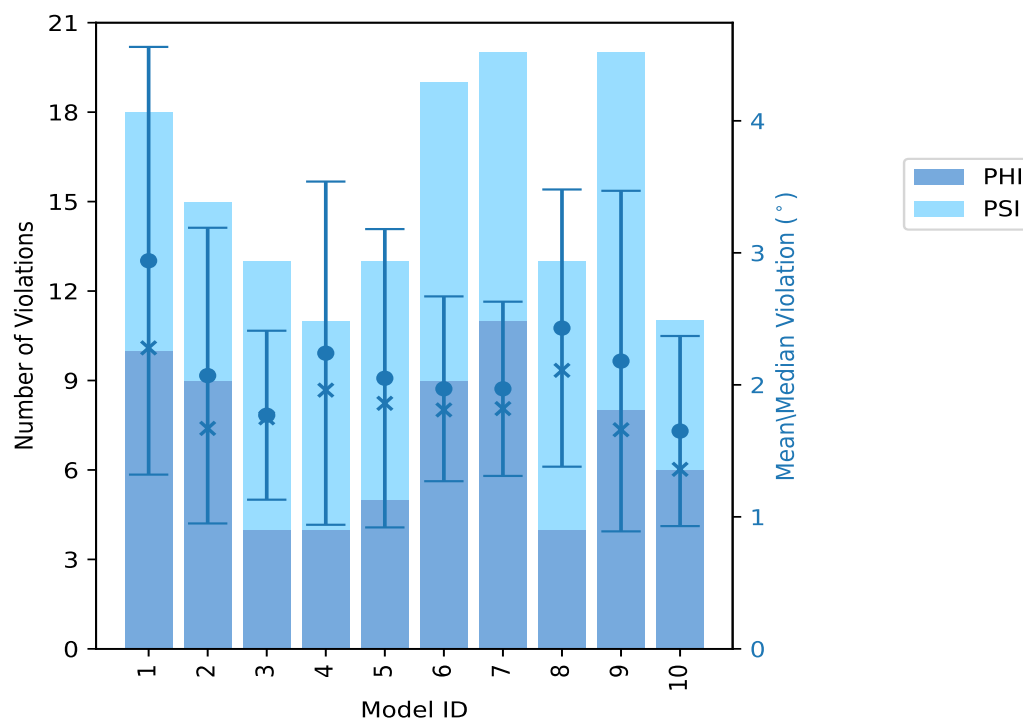
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	10	8	18	2.94	6.68	1.62	2.28
2	9	6	15	2.07	5.66	1.12	1.67
3	4	9	13	1.77	3.59	0.64	1.75
4	4	7	11	2.24	5.74	1.3	1.96
5	5	8	13	2.05	4.58	1.13	1.86
6	9	10	19	1.97	4.02	0.7	1.81
7	11	9	20	1.97	3.24	0.66	1.82
8	4	9	13	2.43	5.04	1.05	2.11
9	8	12	20	2.18	6.03	1.29	1.66
10	6	5	11	1.65	3.56	0.72	1.36

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



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

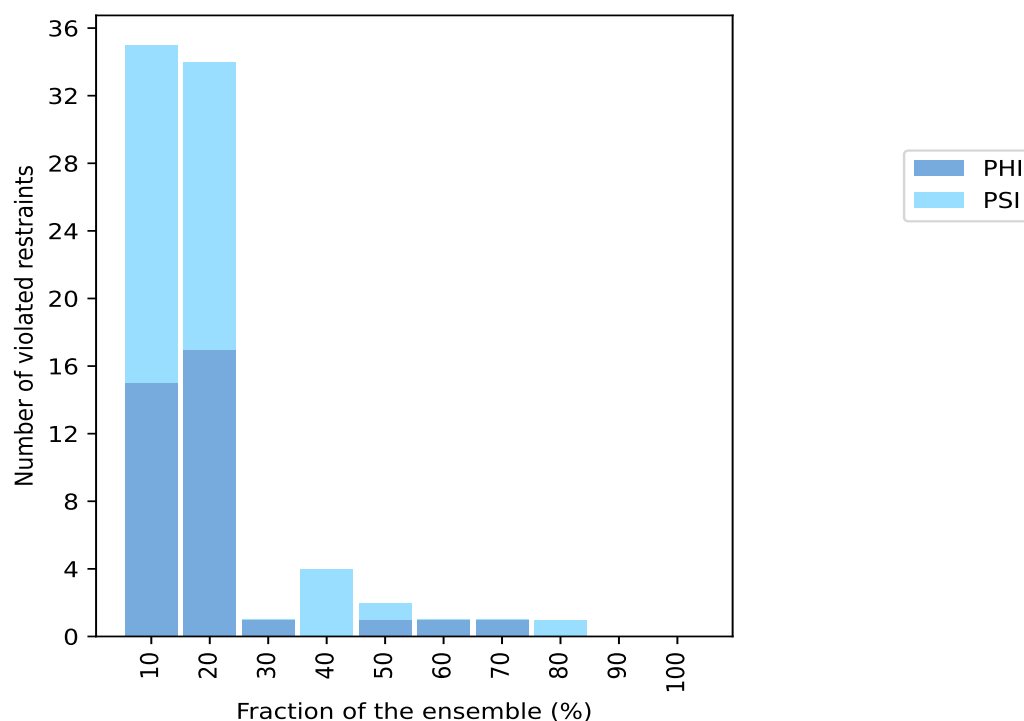
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
15	20	35	1	10.0
17	17	34	2	20.0
1	0	1	3	30.0
0	4	4	4	40.0
1	1	2	5	50.0
1	0	1	6	60.0
1	0	1	7	70.0
0	1	1	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

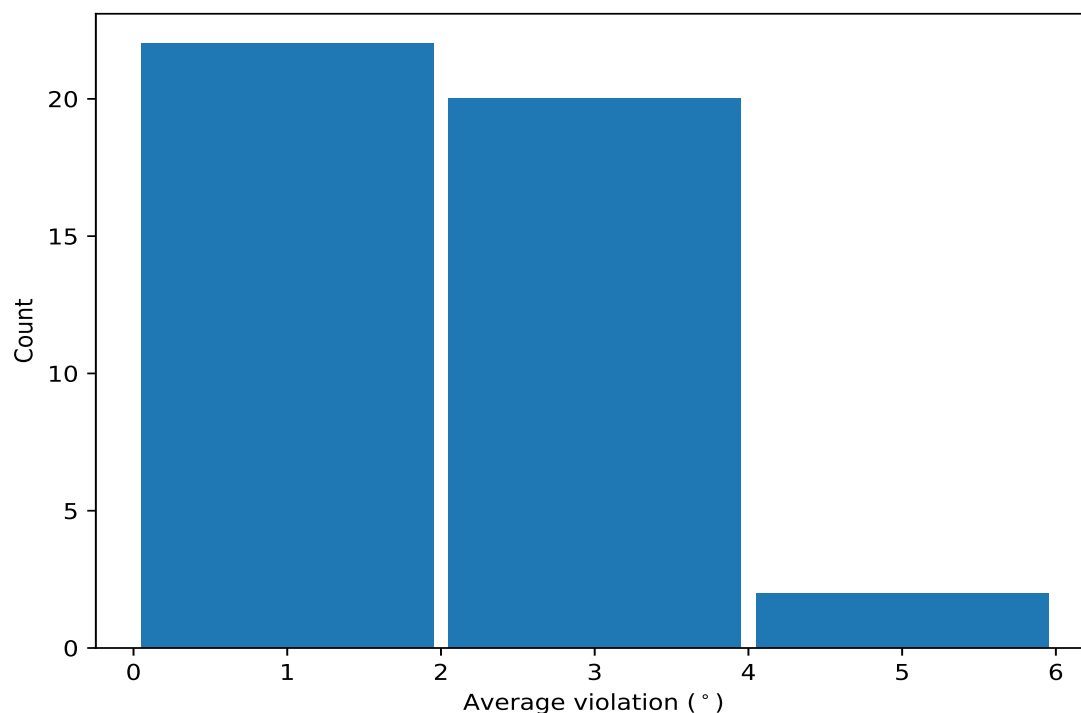
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	8	1.84	0.48	1.86
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	7	3.2	0.8	2.93
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	6	3.74	0.98	3.79
(1,279)	1:223:A:GLU:C	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	5	2.54	2.08	1.66
(1,220)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	5	1.86	0.12	1.85
(1,276)	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	1:223:A:GLU:N	4	2.43	0.83	2.14
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	4	2.12	0.93	1.95
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	4	2.11	0.83	2.04
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	4	1.98	0.95	1.58
(1,285)	1:228:A:LYS:C	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	3	1.49	0.38	1.47
(1,207)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	2	4.36	1.67	4.36
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	2	4.0	0.76	4.0
(1,278)	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	1:224:A:LYS:N	2	3.96	1.2	3.96

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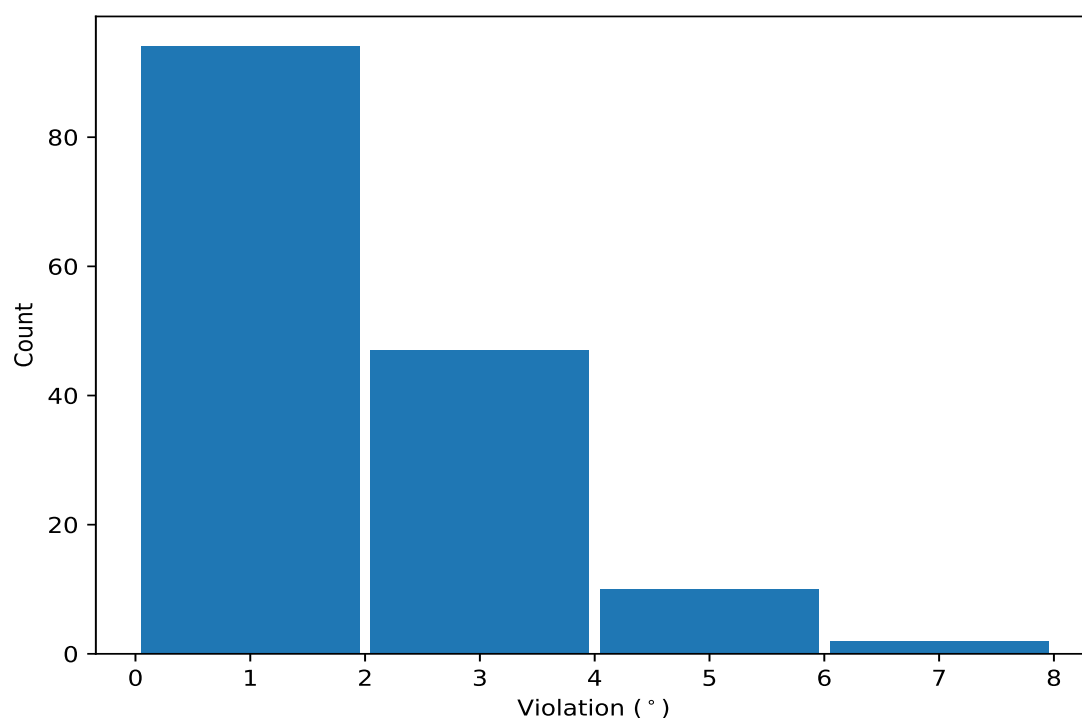
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,201)	1:172:A:VAL:N	1:172:A:VAL:CA	1:172:A:VAL:C	1:173:A:ARG:N	2	3.71	1.33	3.71
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	2	3.43	2.23	3.43
(1,284)	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	1:227:A:ASP:N	2	3.21	1.02	3.21
(1,177)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	2	2.85	1.1	2.85
(1,138)	1:126:A:ALA:C	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	2	2.79	0.26	2.79
(1,210)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	2	2.46	1.16	2.46
(1,208)	1:175:A:ASP:C	1:176:A:THR:N	1:176:A:THR:CA	1:176:A:THR:C	2	2.22	1.0	2.22
(1,296)	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	1:235:A:ALA:N	2	2.2	0.22	2.2
(1,106)	1:97:A:GLY:C	1:98:A:MET:N	1:98:A:MET:CA	1:98:A:MET:C	2	2.19	0.12	2.19
(1,225)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	2	2.18	0.88	2.18
(1,26)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:ASN:N	2	2.16	0.47	2.16
(1,280)	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	1:225:A:GLU:N	2	2.16	0.45	2.16
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	2	2.08	0.57	2.08
(1,283)	1:225:A:GLU:C	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	2	1.95	0.01	1.95
(1,102)	1:92:A:VAL:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	2	1.94	0.85	1.94
(1,212)	1:182:A:ARG:N	1:182:A:ARG:CA	1:182:A:ARG:C	1:183:A:GLY:N	2	1.86	0.29	1.86
(1,85)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	2	1.76	0.05	1.76
(1,76)	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1:78:A:ILE:N	2	1.71	0.32	1.71
(1,218)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:VAL:N	2	1.58	0.52	1.58
(1,71)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	2	1.58	0.07	1.58
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	2	1.43	0.28	1.43
(1,183)	1:159:A:GLN:N	1:159:A:GLN:CA	1:159:A:GLN:C	1:160:A:TYR:N	2	1.42	0.36	1.42
(1,195)	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1:170:A:PHE:N	2	1.41	0.25	1.41
(1,93)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	2	1.39	0.11	1.39
(1,180)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	2	1.3	0.05	1.3
(1,291)	1:231:A:SER:C	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	2	1.29	0.2	1.29
(1,209)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	2	1.28	0.14	1.28
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	2	1.27	0.21	1.27
(1,113)	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	1:102:A:ASP:N	2	1.21	0.18	1.21
(1,196)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	2	1.2	0.04	1.2
(1,215)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	2	1.2	0.08	1.2

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 (°)
(1,279)	1:223:A:GLU:C	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	1	6.68
(1,207)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	9	6.03
(1,199)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	4	5.74
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	2	5.66
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	1	5.18
(1,278)	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	1:224:A:LYS:N	1	5.16
(1,201)	1:172:A:VAL:N	1:172:A:VAL:CA	1:172:A:VAL:C	1:173:A:ARG:N	8	5.04
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1	4.76
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	9	4.75
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	5	4.58
(1,284)	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	1:227:A:ASP:N	5	4.23
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	6	4.02
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1	3.99
(1,177)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	9	3.95
(1,276)	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	1:223:A:GLU:N	1	3.74
(1,210)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	8	3.62
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	3	3.59
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	8	3.58
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	10	3.56
(1,139)	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	1:128:A:ILE:N	1	3.44
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	1	3.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	7	3.24
(1,208)	1:175:A:ASP:C	1:176:A:THR:N	1:176:A:THR:CA	1:176:A:THR:C	9	3.21
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	2	3.1
(1,225)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	2	3.06
(1,138)	1:126:A:ALA:C	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	7	3.05
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	7	2.93
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	4	2.86
(1,102)	1:92:A:VAL:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	7	2.79
(1,278)	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	1:224:A:LYS:N	6	2.76
(1,207)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	6	2.69
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	6	2.67
(1,175)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:HIS:N	4	2.67
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	4	2.65
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	8	2.64
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	4	2.64
(1,26)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:ASN:N	5	2.62
(1,280)	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	1:225:A:GLU:N	7	2.6
(1,276)	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	1:223:A:GLU:N	8	2.57
(1,138)	1:126:A:ALA:C	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	6	2.53
(1,205)	1:174:A:THR:N	1:174:A:THR:CA	1:174:A:THR:C	1:175:A:ASP:N	1	2.46
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	7	2.45
(1,296)	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	1:235:A:ALA:N	9	2.42
(1,201)	1:172:A:VAL:N	1:172:A:VAL:CA	1:172:A:VAL:C	1:173:A:ARG:N	5	2.38
(1,179)	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1:156:A:ASP:N	7	2.38
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	10	2.31
(1,106)	1:97:A:GLY:C	1:98:A:MET:N	1:98:A:MET:CA	1:98:A:MET:C	2	2.31
(1,295)	1:233:A:ASP:C	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	9	2.28
(1,284)	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	1:227:A:ASP:N	6	2.19
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	9	2.15
(1,212)	1:182:A:ARG:N	1:182:A:ARG:CA	1:182:A:ARG:C	1:183:A:GLY:N	8	2.15
(1,70)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:LYS:N	3	2.12
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	8	2.11
(1,218)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:VAL:N	5	2.1
(1,1)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1	2.09
(1,106)	1:97:A:GLY:C	1:98:A:MET:N	1:98:A:MET:CA	1:98:A:MET:C	7	2.07
(1,76)	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1:78:A:ILE:N	3	2.03
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	3	2.02
(1,220)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	5	2.0
(1,296)	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	1:235:A:ALA:N	1	1.98
(1,281)	1:224:A:LYS:C	1:225:A:GLU:N	1:225:A:GLU:CA	1:225:A:GLU:C	8	1.98
(1,285)	1:228:A:LYS:C	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	6	1.97
(1,220)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	7	1.97
(1,283)	1:225:A:GLU:C	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	10	1.96
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	4	1.96
(1,104)	1:93:A:ASP:C	1:94:A:THR:N	1:94:A:THR:CA	1:94:A:THR:C	1	1.95
(1,283)	1:225:A:GLU:C	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	6	1.94
(1,123)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	2	1.94
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	7	1.92
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	1	1.87
(1,116)	1:102:A:ASP:C	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	8	1.87
(1,279)	1:223:A:GLU:C	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	5	1.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,220)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	8	1.85
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	6	1.85
(1,220)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	6	1.81
(1,85)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	3	1.81
(1,152)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:TYR:N	9	1.8
(1,183)	1:159:A:GLN:N	1:159:A:GLN:CA	1:159:A:GLN:C	1:160:A:TYR:N	3	1.79
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	3	1.75
(1,177)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	6	1.75
(1,62)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:SER:N	3	1.73
(1,276)	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	1:223:A:GLU:N	6	1.72
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	2	1.72
(1,280)	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	1:225:A:GLU:N	9	1.71
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	10	1.71
(1,85)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	7	1.71
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	2	1.71
(1,276)	1:222:A:VAL:N	1:222:A:VAL:CA	1:222:A:VAL:C	1:223:A:GLU:N	10	1.7
(1,26)	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	1:40:A:ASN:N	3	1.69
(1,220)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	2	1.67
(1,190)	1:162:A:TRP:C	1:163:A:GLU:N	1:163:A:GLU:CA	1:163:A:GLU:C	2	1.67
(1,279)	1:223:A:GLU:C	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	8	1.66
(1,195)	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1:170:A:PHE:N	9	1.66
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	9	1.66
(1,71)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	6	1.65
(1,165)	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	1:149:A:THR:N	7	1.61
(1,137)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:ASP:N	7	1.61
(1,154)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:TYR:N	2	1.6
(1,23)	1:34:A:ILE:C	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	6	1.59
(1,212)	1:182:A:ARG:N	1:182:A:ARG:CA	1:182:A:ARG:C	1:183:A:GLY:N	9	1.56
(1,182)	1:158:A:GLU:C	1:159:A:GLN:N	1:159:A:GLN:CA	1:159:A:GLN:C	2	1.53
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	2	1.51
(1,93)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	1	1.5
(1,71)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	9	1.5
(1,291)	1:231:A:SER:C	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	9	1.49
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	7	1.49
(1,285)	1:228:A:LYS:C	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	7	1.47
(1,279)	1:223:A:GLU:C	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	6	1.46
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	8	1.46
(1,184)	1:159:A:GLN:C	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	1	1.43
(1,209)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	4	1.42
(1,8)	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	1:22:A:PHE:N	6	1.4
(1,113)	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	1:102:A:ASP:N	9	1.39
(1,76)	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1:78:A:ILE:N	9	1.39
(1,211)	1:181:A:GLY:C	1:182:A:ARG:N	1:182:A:ARG:CA	1:182:A:ARG:C	10	1.36
(1,193)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:SER:N	7	1.36
(1,180)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	2	1.35
(1,29)	1:43:A:ILE:C	1:44:A:PHE:N	1:44:A:PHE:CA	1:44:A:PHE:C	7	1.34
(1,225)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	6	1.31
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	9	1.29
(1,210)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	7	1.29
(1,215)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	4	1.28
(1,93)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	3	1.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,180)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1	1.25
(1,196)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	9	1.24
(1,208)	1:175:A:ASP:C	1:176:A:THR:N	1:176:A:THR:CA	1:176:A:THR:C	5	1.22
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	5	1.2
(1,82)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:ILE:N	5	1.2
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	10	1.18
(1,196)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	5	1.17
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	4	1.17
(1,298)	1:236:A:GLU:N	1:236:A:GLU:CA	1:236:A:GLU:C	1:237:A:GLU:N	4	1.16
(1,195)	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1:170:A:PHE:N	2	1.16
(1,209)	1:179:A:PRO:C	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	7	1.15
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	3	1.15
(1,215)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	10	1.12
(1,291)	1:231:A:SER:C	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	1	1.09
(1,233)	1:192:A:GLU:C	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	10	1.09
(1,102)	1:92:A:VAL:C	1:93:A:ASP:N	1:93:A:ASP:CA	1:93:A:ASP:C	1	1.09
(1,234)	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	1:194:A:GLN:N	10	1.07
(1,218)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:VAL:N	4	1.07
(1,279)	1:223:A:GLU:C	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	3	1.06
(1,183)	1:159:A:GLN:N	1:159:A:GLN:CA	1:159:A:GLN:C	1:160:A:TYR:N	10	1.06
(1,109)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:LYS:N	9	1.06
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	2	1.06
(1,150)	1:135:A:GLY:C	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	9	1.04
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:THR:N	6	1.04
(1,285)	1:228:A:LYS:C	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	3	1.03
(1,113)	1:101:A:ALA:N	1:101:A:ALA:CA	1:101:A:ALA:C	1:102:A:ASP:N	5	1.03
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	6	1.02
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	5	1.02
(1,110)	1:99:A:THR:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	7	1.02
(1,214)	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1:184:A:THR:N	8	1.0