



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 11:47 AM UTC

PDB ID : 8JR7 / pdb_00008jr7
BMRB ID : 36576
Title : N-terminal domain of Hsp90 mutant
Authors : Wan, C.J.
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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

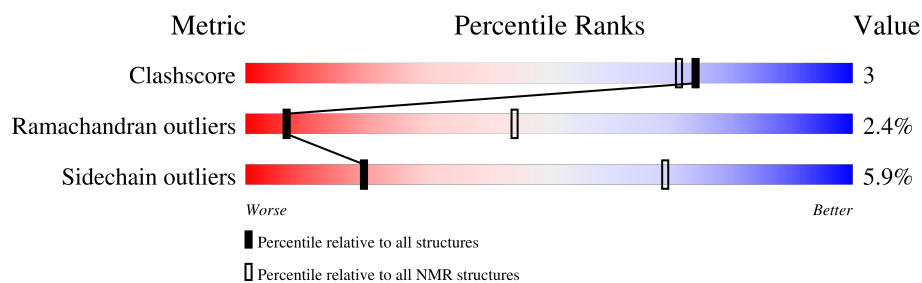
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	237	 77% • 20%

2 Ensemble composition and analysis

This entry contains 10 models. Model 9 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:17-A:62, A:76-A:110, A:115-A:223 (190)	2.10	9

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, 5, 8, 9, 10
2	6, 7

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3718 atoms, of which 1840 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
			3718	1177	1840	306	388	7	

There is a discrepancy between the modelled and reference sequences:

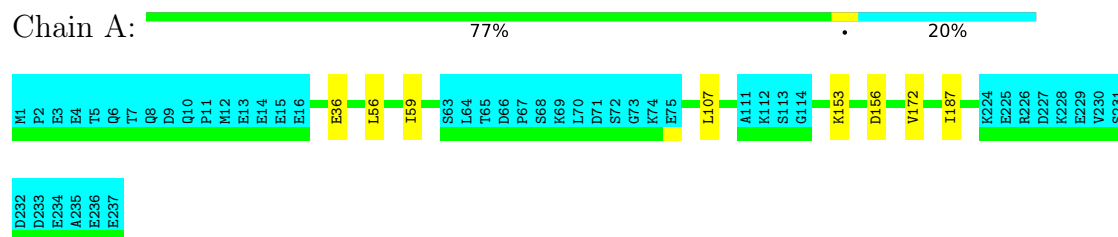
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLU	THR	engineered mutation	UNP P07900

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

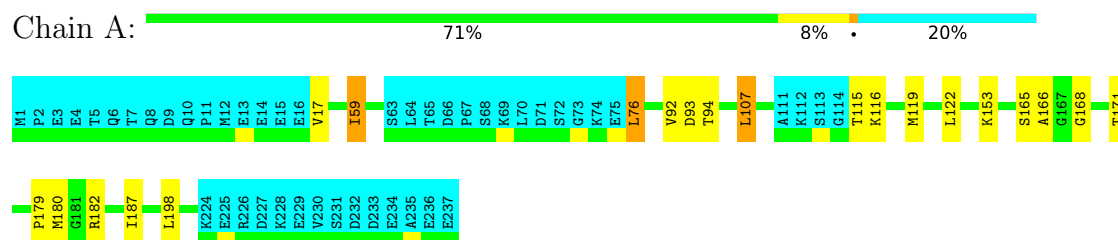


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

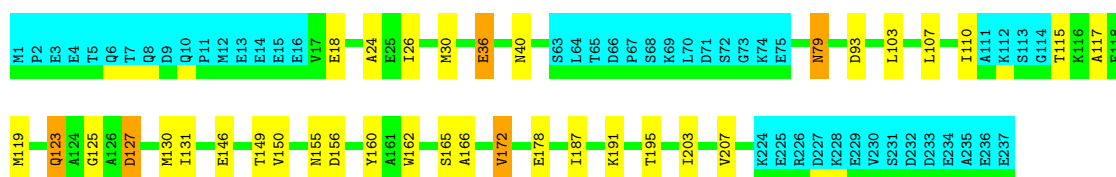
- Molecule 1: Heat shock protein HSP 90-alpha



4.2.2 Score per residue for model 2

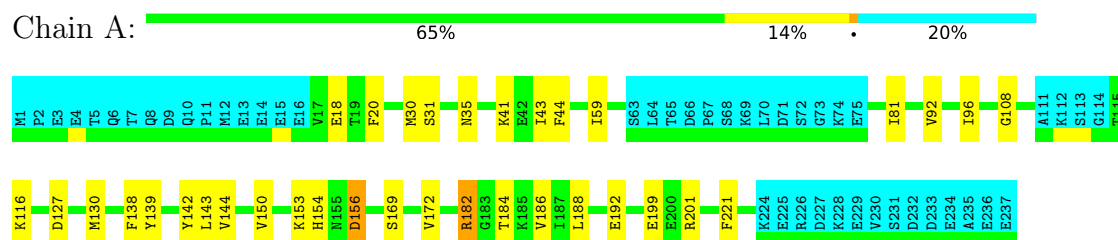
- Molecule 1: Heat shock protein HSP 90-alpha





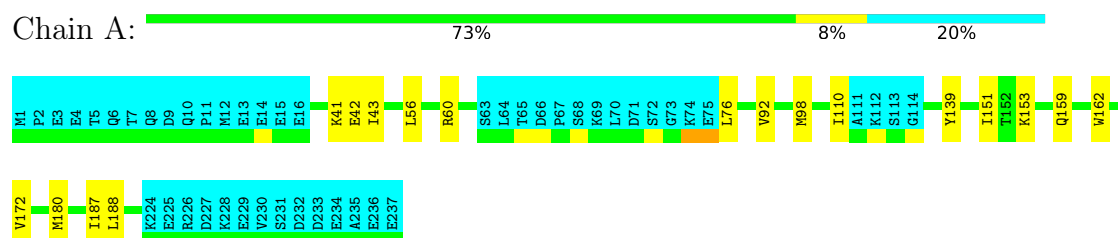
4.2.3 Score per residue for model 3

- Molecule 1: Heat shock protein HSP 90-alpha



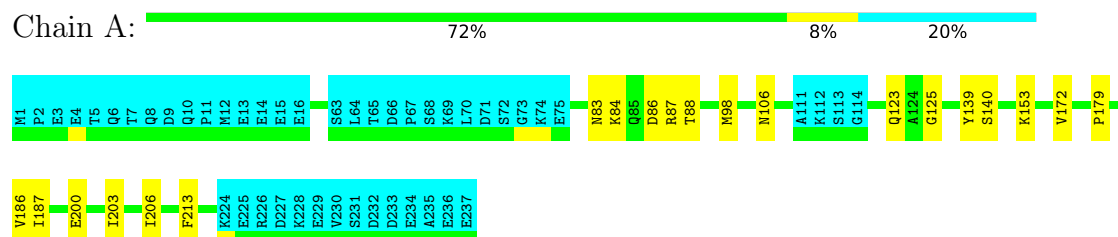
4.2.4 Score per residue for model 4

- Molecule 1: Heat shock protein HSP 90-alpha



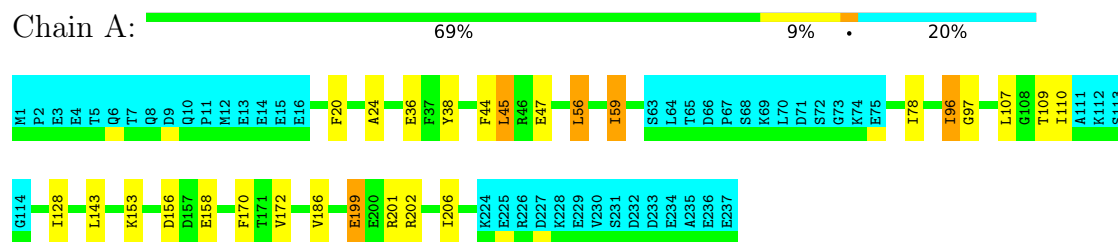
4.2.5 Score per residue for model 5

- Molecule 1: Heat shock protein HSP 90-alpha



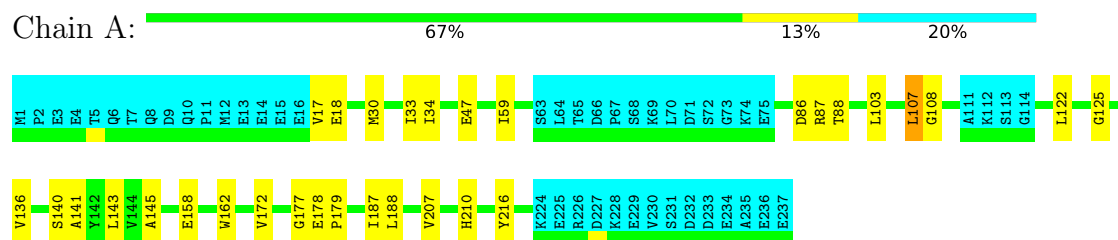
4.2.6 Score per residue for model 6

- Molecule 1: Heat shock protein HSP 90-alpha



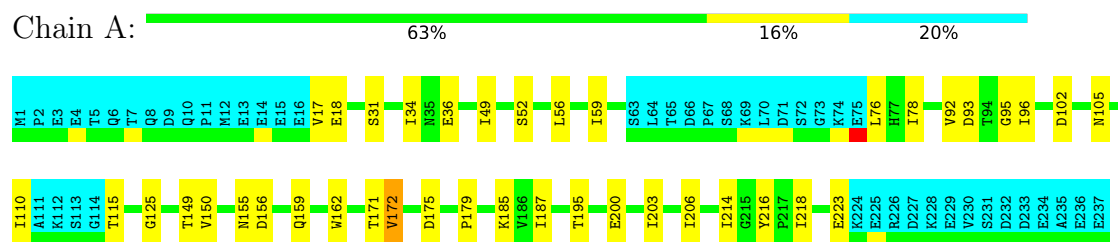
4.2.7 Score per residue for model 7

- Molecule 1: Heat shock protein HSP 90-alpha



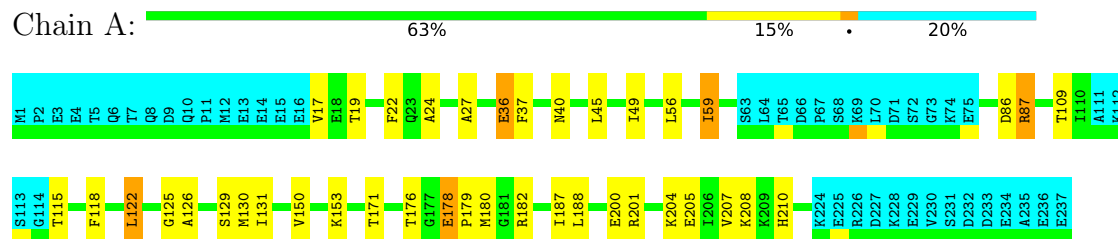
4.2.8 Score per residue for model 8

- Molecule 1: Heat shock protein HSP 90-alpha



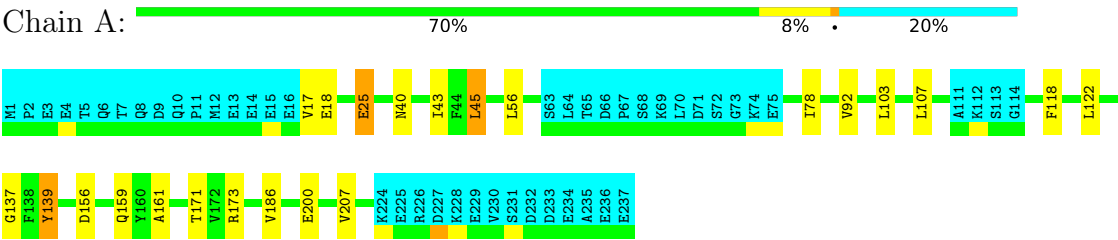
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Heat shock protein HSP 90-alpha



4.2.10 Score per residue for model 10

- Molecule 1: Heat shock protein HSP 90-alpha



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	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	464
Number of shifts mapped to atoms	464
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 [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.66±0.03	0±0/1535 (0.0± 0.0%)	0.71±0.02	0±0/2073 (0.0± 0.0%)
All	All	0.66	2/15350 (0.0%)	0.71	0/20730 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	172	VAL	CA-CB	5.99	1.61	1.54	2	1
1	A	178	GLU	C-N	5.15	1.39	1.34	9	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1509	1508	1508	10±3
All	All	15090	15080	15080	96

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:153:LYS:HB2	1:A:180:MET:SD	0.62	2.35	9	1
1:A:107:LEU:O	1:A:107:LEU:HG	0.59	1.97	1	1
1:A:103:LEU:O	1:A:107:LEU:HB3	0.58	1.98	10	1
1:A:83:ASN:O	1:A:88:THR:HB	0.57	2.00	5	1
1:A:31:SER:O	1:A:35:ASN:HB2	0.56	2.00	3	1
1:A:22:PHE:CD1	1:A:27:ALA:HB2	0.55	2.36	9	1
1:A:78:ILE:HD12	1:A:216:TYR:CE1	0.54	2.38	8	1
1:A:107:LEU:HD21	1:A:162:TRP:CZ2	0.53	2.37	7	1
1:A:204:LYS:O	1:A:208:LYS:HB2	0.53	2.03	9	1
1:A:187:ILE:O	1:A:187:ILE:HG13	0.53	2.04	5	1
1:A:153:LYS:HD3	1:A:180:MET:O	0.52	2.03	1	1
1:A:153:LYS:HB2	1:A:180:MET:CG	0.52	2.34	4	1
1:A:207:VAL:HA	1:A:210:HIS:CE1	0.52	2.40	7	2
1:A:31:SER:O	1:A:34:ILE:HG22	0.52	2.04	8	1
1:A:18:GLU:HB2	1:A:172:VAL:O	0.52	2.05	8	1
1:A:185:LYS:N	1:A:185:LYS:HD2	0.52	2.20	8	1
1:A:153:LYS:O	1:A:182:ARG:HA	0.51	2.04	1	2
1:A:214:ILE:HG21	1:A:218:ILE:HD11	0.51	1.82	8	1
1:A:199:GLU:OE1	1:A:201:ARG:HB2	0.51	2.05	3	2
1:A:154:HIS:CD2	1:A:156:ASP:HB3	0.51	2.40	3	1
1:A:153:LYS:CG	1:A:179:PRO:HA	0.51	2.36	5	1
1:A:30:MET:O	1:A:34:ILE:HG12	0.51	2.06	7	1
1:A:115:THR:HB	1:A:119:MET:SD	0.50	2.46	1	1
1:A:155:ASN:O	1:A:156:ASP:HB3	0.50	2.06	2	2
1:A:52:SER:OG	1:A:78:ILE:HD11	0.50	2.06	8	1
1:A:151:ILE:HB	1:A:159:GLN:OE1	0.50	2.07	4	1
1:A:102:ASP:HA	1:A:105:ASN:ND2	0.50	2.21	8	1
1:A:150:VAL:HG23	1:A:162:TRP:HB3	0.49	1.82	8	1
1:A:162:TRP:CE3	1:A:172:VAL:HB	0.49	2.42	4	2
1:A:45:LEU:O	1:A:49:ILE:HG12	0.49	2.08	9	1
1:A:127:ASP:OD1	1:A:130:MET:HB2	0.49	2.07	2	2
1:A:44:PHE:CE1	1:A:143:LEU:HD12	0.49	2.43	6	1
1:A:115:THR:O	1:A:119:MET:HB2	0.49	2.08	2	1
1:A:25:GLU:H	1:A:25:GLU:CD	0.48	2.14	10	1
1:A:81:ILE:HG22	1:A:221:PHE:O	0.48	2.08	3	1
1:A:118:PHE:O	1:A:122:LEU:HG	0.48	2.08	10	1
1:A:30:MET:O	1:A:33:ILE:HG22	0.48	2.08	7	1
1:A:86:ASP:O	1:A:87:ARG:HG2	0.48	2.09	9	1
1:A:86:ASP:O	1:A:88:THR:HG23	0.47	2.10	7	1
1:A:79:ASN:HD22	1:A:79:ASN:N	0.46	2.08	2	1
1:A:41:LYS:C	1:A:43:ILE:H	0.46	2.18	4	2
1:A:56:LEU:O	1:A:60:ARG:HG2	0.46	2.09	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ASP:C	1:A:87:ARG:HD3	0.46	2.36	7	1
1:A:45:LEU:HD11	1:A:207:VAL:HG12	0.45	1.87	10	1
1:A:150:VAL:HB	1:A:162:TRP:HB3	0.45	1.86	2	1
1:A:140:SER:O	1:A:143:LEU:HB2	0.45	2.10	7	1
1:A:56:LEU:O	1:A:59:ILE:HG22	0.45	2.11	6	1
1:A:59:ILE:HG12	1:A:76:LEU:HD13	0.45	1.87	1	1
1:A:115:THR:O	1:A:116:LYS:HG3	0.45	2.12	1	1
1:A:115:THR:HA	1:A:118:PHE:CE2	0.44	2.47	9	1
1:A:161:ALA:O	1:A:173:ARG:HG2	0.44	2.12	10	1
1:A:159:GLN:OE1	1:A:179:PRO:HA	0.44	2.12	8	1
1:A:203:ILE:O	1:A:206:ILE:HG22	0.44	2.13	5	2
1:A:137:GLY:C	1:A:139:TYR:H	0.44	2.21	10	1
1:A:20:PHE:HB3	1:A:170:PHE:CZ	0.44	2.47	6	1
1:A:139:TYR:CG	1:A:140:SER:N	0.44	2.86	5	1
1:A:38:TYR:CE1	1:A:128:ILE:HD12	0.44	2.47	6	1
1:A:18:GLU:O	1:A:171:THR:HA	0.43	2.13	10	1
1:A:96:ILE:HG23	1:A:97:GLY:N	0.43	2.27	6	1
1:A:45:LEU:HG	1:A:206:ILE:HG22	0.43	1.90	6	1
1:A:138:PHE:CE1	1:A:143:LEU:HB2	0.43	2.49	3	1
1:A:59:ILE:CD1	1:A:95:GLY:HA2	0.43	2.43	8	1
1:A:177:GLY:O	1:A:179:PRO:HD3	0.43	2.13	7	1
1:A:103:LEU:HD22	1:A:160:TYR:CE1	0.42	2.49	2	1
1:A:122:LEU:HD23	1:A:126:ALA:HA	0.42	1.90	9	1
1:A:200:GLU:O	1:A:204:LYS:HG2	0.42	2.14	9	1
1:A:18:GLU:HB2	1:A:172:VAL:HG13	0.42	1.89	3	1
1:A:178:GLU:N	1:A:179:PRO:CD	0.42	2.83	9	1
1:A:36:GLU:HG3	1:A:37:PHE:H	0.42	1.74	9	1
1:A:44:PHE:CB	1:A:143:LEU:HD11	0.41	2.45	3	1
1:A:146:GLU:HG3	1:A:191:LYS:HD3	0.41	1.92	2	1
1:A:56:LEU:HA	1:A:59:ILE:CG2	0.41	2.45	9	1
1:A:84:LYS:C	1:A:86:ASP:N	0.41	2.79	5	1
1:A:214:ILE:HG23	1:A:216:TYR:CE2	0.41	2.50	8	1
1:A:146:GLU:O	1:A:165:SER:HB3	0.41	2.16	2	1
1:A:30:MET:HE2	1:A:142:TYR:CE1	0.41	2.51	3	1
1:A:44:PHE:HB2	1:A:143:LEU:HD11	0.41	1.93	3	1
1:A:202:ARG:O	1:A:206:ILE:HG12	0.41	2.16	6	1
1:A:141:ALA:O	1:A:145:ALA:HB3	0.41	2.16	7	1
1:A:201:ARG:O	1:A:205:GLU:HG3	0.41	2.16	9	1
1:A:123:GLN:HE21	1:A:123:GLN:HA	0.41	1.76	2	1
1:A:182:ARG:HG3	1:A:182:ARG:O	0.40	2.16	1	1
1:A:203:ILE:O	1:A:207:VAL:HG22	0.40	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PHE:O	1:A:169:SER:HA	0.40	2.16	3	1
1:A:129:SER:C	1:A:131:ILE:H	0.40	2.24	9	1
1:A:40:ASN:O	1:A:43:ILE:HG22	0.40	2.16	10	1
1:A:76:LEU:HG	1:A:94:THR:HB	0.40	1.93	1	1
1:A:146:GLU:CG	1:A:191:LYS:HD3	0.40	2.46	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	190/237 (80%)	165±5 (87±3%)	20±5 (11±3%)	5±2 (2±1%)	7	44
All	All	1900/2370 (80%)	1649 (87%)	205 (11%)	46 (2%)	7	44

All 24 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	17	VAL	5
1	A	125	GLY	5
1	A	36	GLU	4
1	A	24	ALA	3
1	A	139	TYR	3
1	A	156	ASP	3
1	A	166	ALA	2
1	A	40	ASN	2
1	A	110	ILE	2
1	A	108	GLY	2
1	A	107	LEU	2
1	A	165	SER	1
1	A	168	GLY	1
1	A	179	PRO	1
1	A	117	ALA	1
1	A	144	VAL	1
1	A	42	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	87	ARG	1
1	A	213	PHE	1
1	A	96	ILE	1
1	A	158	GLU	1
1	A	136	VAL	1
1	A	109	THR	1
1	A	130	MET	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	164/207 (79%)	154±3 (94±2%)	10±3 (6±2%)	19	69
All	All	1640/2070 (79%)	1543 (94%)	97 (6%)	19	69

All 49 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	187	ILE	6
1	A	59	ILE	5
1	A	92	VAL	5
1	A	172	VAL	5
1	A	186	VAL	4
1	A	188	LEU	4
1	A	76	LEU	3
1	A	122	LEU	3
1	A	171	THR	3
1	A	200	GLU	3
1	A	56	LEU	3
1	A	93	ASP	2
1	A	107	LEU	2
1	A	18	GLU	2
1	A	123	GLN	2
1	A	149	THR	2
1	A	178	GLU	2
1	A	195	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	96	ILE	2
1	A	150	VAL	2
1	A	182	ARG	2
1	A	98	MET	2
1	A	110	ILE	2
1	A	45	LEU	2
1	A	47	GLU	2
1	A	78	ILE	2
1	A	198	LEU	1
1	A	36	GLU	1
1	A	79	ASN	1
1	A	127	ASP	1
1	A	131	ILE	1
1	A	184	THR	1
1	A	192	GLU	1
1	A	106	ASN	1
1	A	109	THR	1
1	A	153	LYS	1
1	A	199	GLU	1
1	A	103	LEU	1
1	A	158	GLU	1
1	A	216	TYR	1
1	A	49	ILE	1
1	A	115	THR	1
1	A	175	ASP	1
1	A	223	GLU	1
1	A	19	THR	1
1	A	87	ARG	1
1	A	176	THR	1
1	A	25	GLU	1
1	A	159	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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	464
Number of shifts mapped to atoms	464
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. 416 atoms were assigned a chemical shift out of a possible 2623. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/957 (0%)	0/390 (0%)	0/380 (0%)	0/187 (0%)
Sidechain	416/1463 (28%)	312/953 (33%)	104/461 (23%)	0/49 (0%)
Aromatic	0/203 (0%)	0/100 (0%)	0/98 (0%)	0/5 (0%)
Overall	416/2623 (16%)	312/1443 (22%)	104/939 (11%)	0/241 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 464 atoms were assigned a chemical shift out of a possible 3199. 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	464/1808 (26%)	348/1167 (30%)	116/581 (20%)	0/60 (0%)
Aromatic	0/203 (0%)	0/100 (0%)	0/98 (0%)	0/5 (0%)
Overall	464/3199 (15%)	348/1750 (20%)	116/1153 (10%)	0/296 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

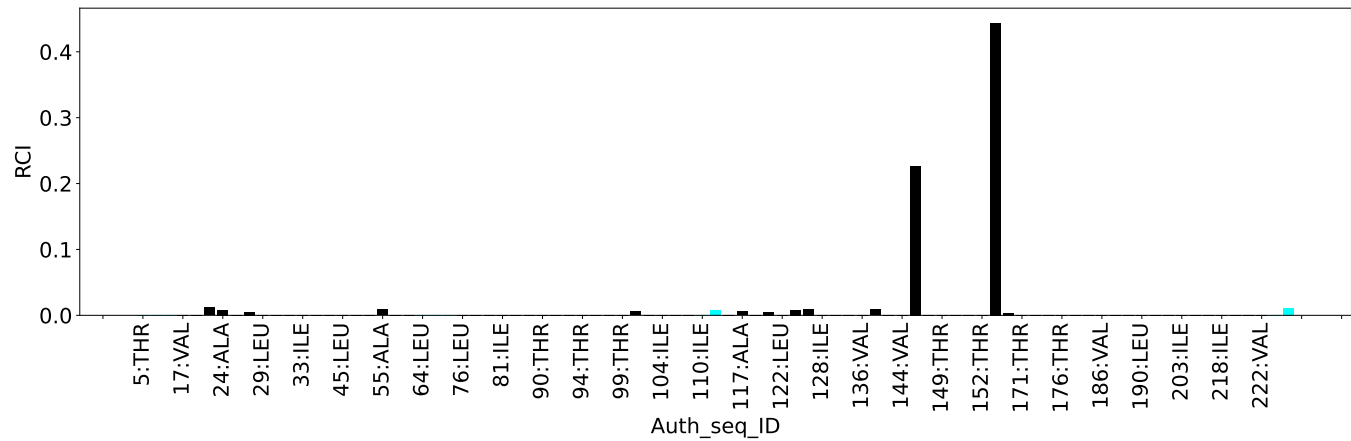
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	107	LEU	HD11	-0.96	-0.61 – 2.12	-6.3
1	A	107	LEU	HD12	-0.96	-0.61 – 2.12	-6.3
1	A	107	LEU	HD13	-0.96	-0.61 – 2.12	-6.3
1	A	144	VAL	CG2	12.69	13.71 – 28.88	-5.7
1	A	144	VAL	HG21	-0.71	-0.58 – 2.19	-5.5
1	A	144	VAL	HG22	-0.71	-0.58 – 2.19	-5.5
1	A	144	VAL	HG23	-0.71	-0.58 – 2.19	-5.5
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	1276
Intra-residue ($ i-j =0$)	104
Sequential ($ i-j =1$)	277
Medium range ($ i-j >1$ and $ i-j <5$)	294
Long range ($ i-j \geq 5$)	451
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)	82.7	0.2
0.2-0.5 (Medium)	45.3	0.5
>0.5 (Large)	1.0	0.88

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)	20.3	8.38
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

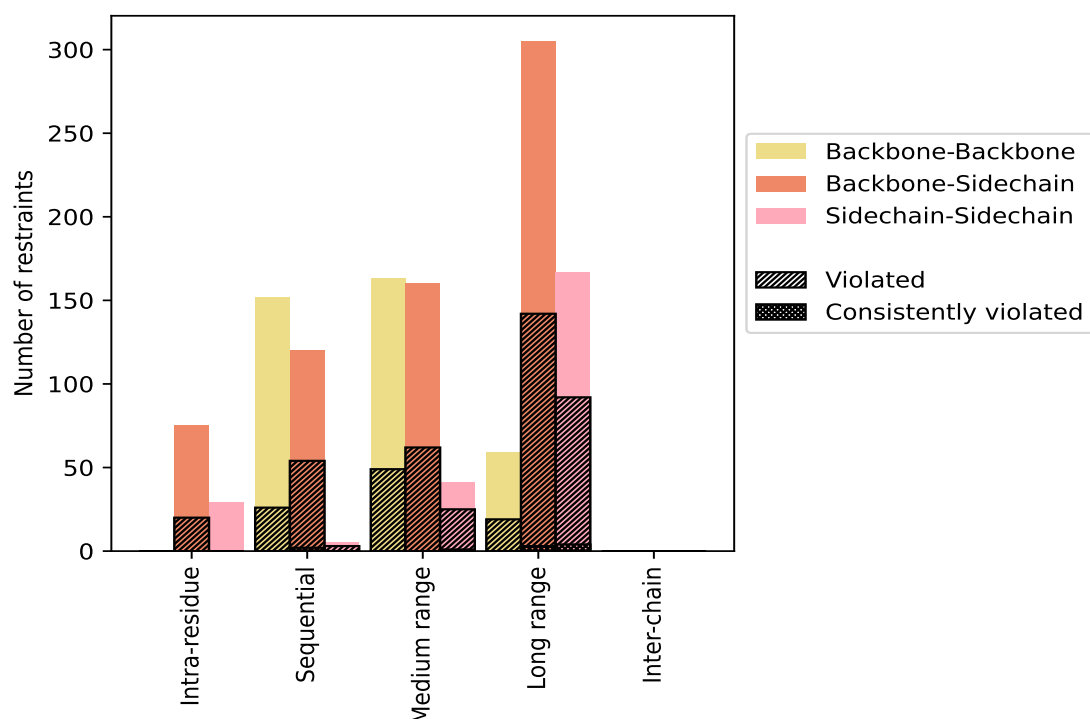
9.1 Summary of distance violations ⓘ

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	20	19.2	1.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	75	5.9	20	26.7	1.6	0	0.0	0.0
Sidechain-Sidechain	29	2.3	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	277	21.7	83	30.0	6.5	2	0.7	0.2
Backbone-Backbone	152	11.9	26	17.1	2.0	0	0.0	0.0
Backbone-Sidechain	120	9.4	54	45.0	4.2	2	1.7	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)	294	23.0	121	41.2	9.5	1	0.3	0.1
Backbone-Backbone	163	12.8	49	30.1	3.8	0	0.0	0.0
Backbone-Sidechain	90	7.1	47	52.2	3.7	0	0.0	0.0
Sidechain-Sidechain	41	3.2	25	61.0	2.0	1	2.4	0.1
Long range (i-j ≥5)	451	35.3	236	52.3	18.5	7	1.6	0.5
Backbone-Backbone	59	4.6	19	32.2	1.5	0	0.0	0.0
Backbone-Sidechain	225	17.6	125	55.6	9.8	3	1.3	0.2
Sidechain-Sidechain	167	13.1	92	55.1	7.2	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	11.8	32	21.3	2.5	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1276	100.0	492	38.6	38.6	10	0.8	0.8
Backbone-Backbone	374	29.3	94	25.1	7.4	0	0.0	0.0
Backbone-Sidechain	660	51.7	278	42.1	21.8	5	0.8	0.4
Sidechain-Sidechain	242	19.0	120	49.6	9.4	5	2.1	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

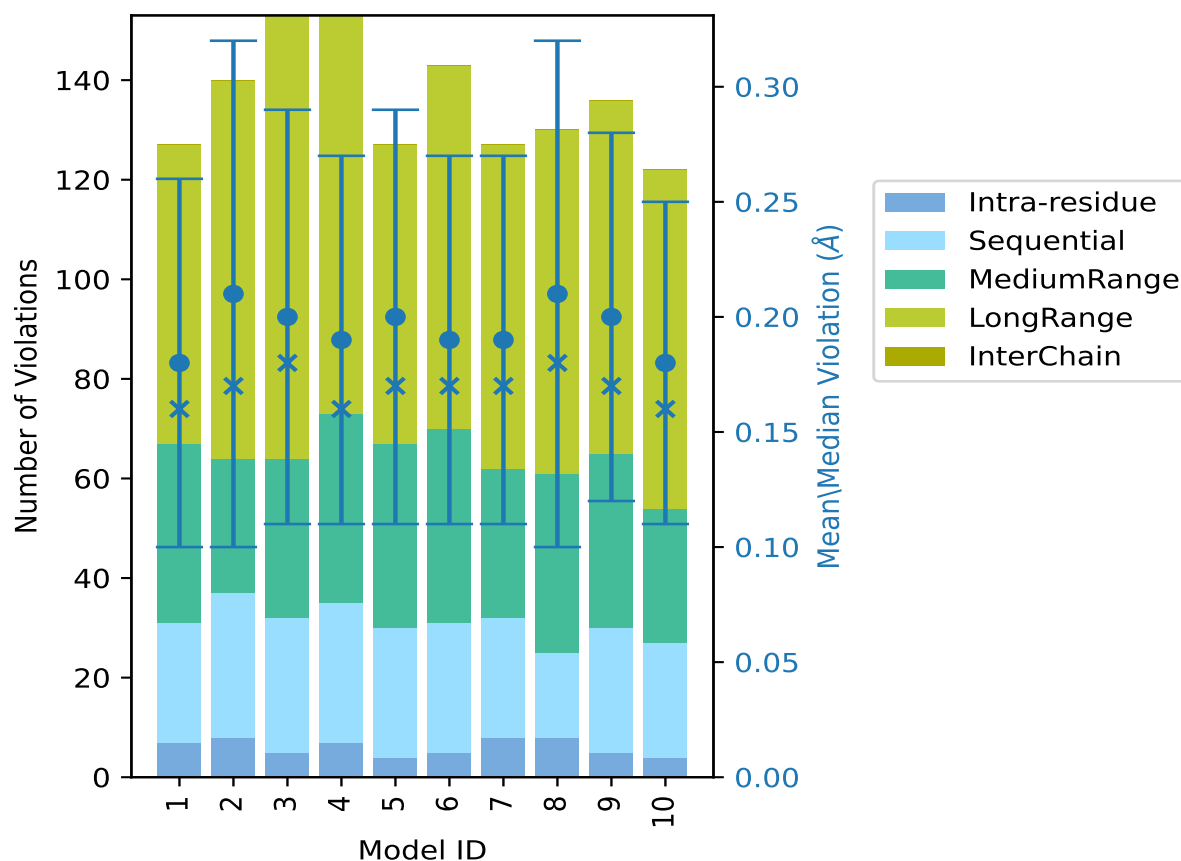
9.2 Distance violation statistics for each model [i](#)

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	7	24	36	60	0	127	0.18	0.47	0.08	0.16
2	8	29	27	76	0	140	0.21	0.79	0.11	0.17
3	5	27	32	89	0	153	0.2	0.57	0.09	0.18
4	7	28	38	80	0	153	0.19	0.45	0.08	0.16
5	4	26	37	60	0	127	0.2	0.57	0.09	0.17
6	5	26	39	73	0	143	0.19	0.51	0.08	0.17
7	8	24	30	65	0	127	0.19	0.55	0.08	0.17
8	8	17	36	69	0	130	0.21	0.88	0.11	0.18
9	5	25	35	71	0	136	0.2	0.52	0.08	0.17
10	4	23	27	68	0	122	0.18	0.43	0.07	0.16

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, 666(IR:84, SQ:194, MR:173, LR:215, 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	%
7	28	46	95	0	176	1	10.0
5	21	36	42	0	104	2	20.0
1	8	9	33	0	51	3	30.0

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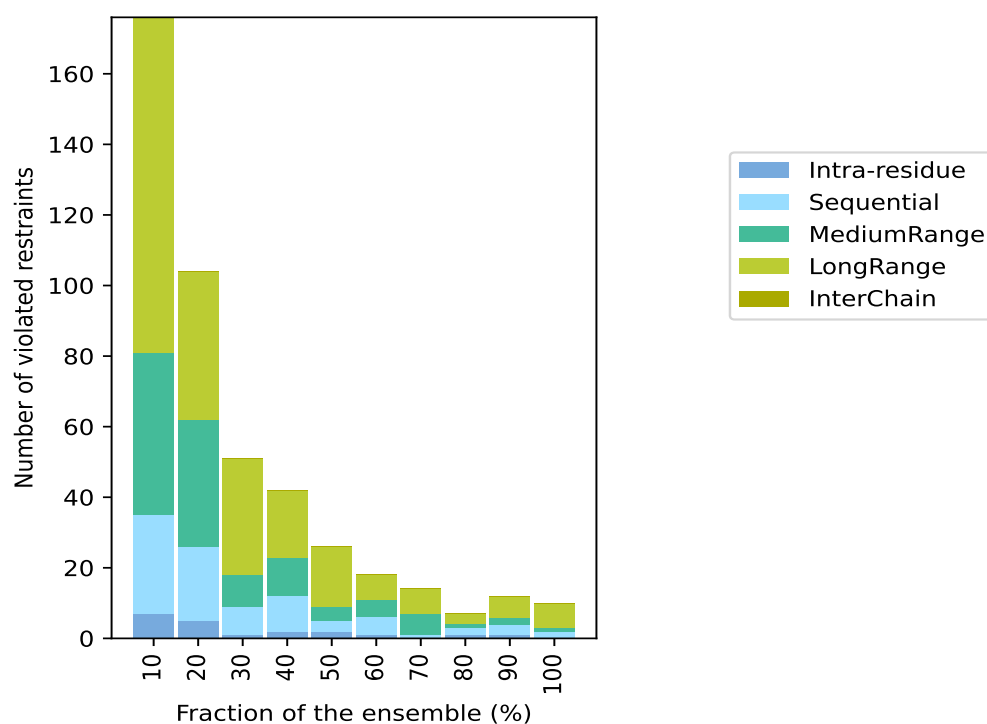
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	10	11	19	0	42	4	40.0
2	3	4	17	0	26	5	50.0
1	5	5	7	0	18	6	60.0
0	1	6	7	0	14	7	70.0
1	2	1	3	0	7	8	80.0
1	3	2	6	0	12	9	90.0
0	2	1	7	0	10	10	100.0

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 ⓘ

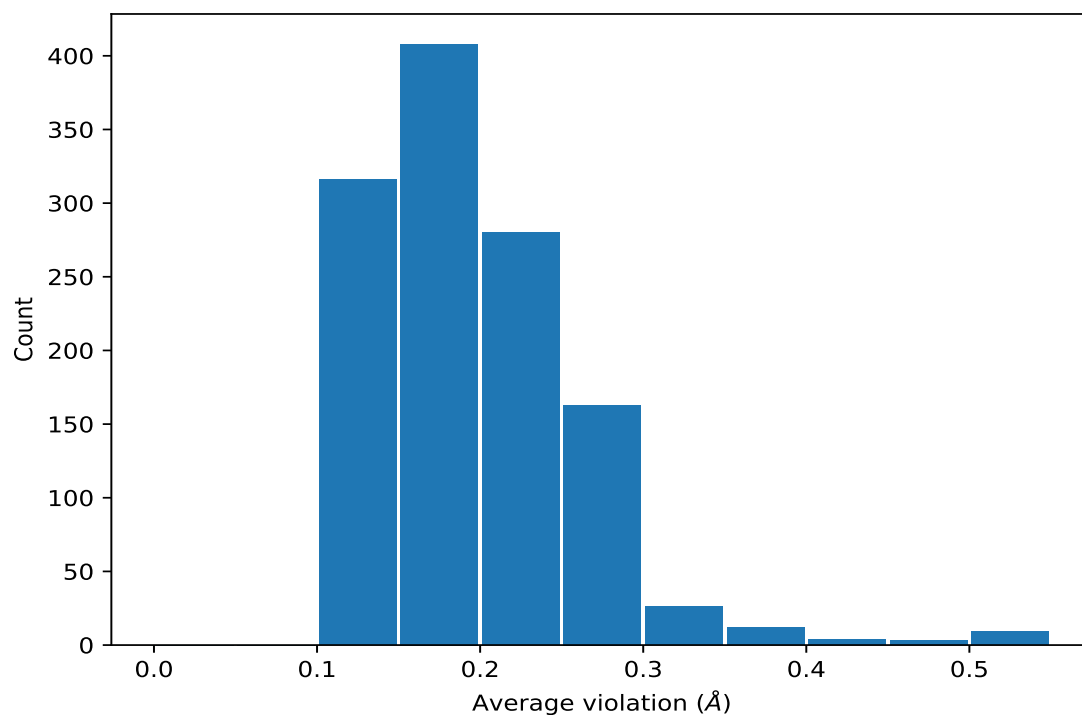


9.4 Most violated distance restraints in the ensemble ⓘ

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)
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	10	0.32	0.1	0.29
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	10	0.32	0.1	0.29
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	10	0.28	0.1	0.28
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	10	0.28	0.1	0.28
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	10	0.28	0.1	0.28
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	10	0.28	0.1	0.28
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	10	0.28	0.1	0.28
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	10	0.28	0.1	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	10	0.28	0.1	0.28
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	10	0.28	0.1	0.28
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	10	0.28	0.1	0.28
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	10	0.28	0.04	0.26
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	10	0.28	0.04	0.26
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	10	0.28	0.04	0.26
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	10	0.26	0.06	0.26
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	10	0.26	0.06	0.26
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	10	0.2	0.04	0.19
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	10	0.2	0.04	0.19
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	10	0.2	0.04	0.19
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	10	0.2	0.07	0.19
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	10	0.2	0.07	0.19
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	10	0.2	0.07	0.19
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	10	0.19	0.06	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	10	0.19	0.06	0.2
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	10	0.18	0.03	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	10	0.18	0.03	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	10	0.18	0.03	0.18
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	10	0.17	0.05	0.17
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	10	0.17	0.05	0.17
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	10	0.17	0.05	0.17
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	10	0.17	0.04	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	10	0.17	0.04	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	10	0.17	0.04	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	10	0.17	0.04	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	10	0.17	0.04	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	10	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	10	0.17	0.04	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	10	0.17	0.04	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	10	0.17	0.04	0.16
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	9	0.36	0.09	0.37
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	9	0.36	0.09	0.37
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	9	0.33	0.09	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	9	0.33	0.09	0.28
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	9	0.28	0.1	0.29
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	9	0.28	0.1	0.29
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	9	0.28	0.1	0.29
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	9	0.24	0.06	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	9	0.24	0.06	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	9	0.24	0.06	0.26
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	9	0.23	0.08	0.21
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	9	0.23	0.08	0.21
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	9	0.22	0.08	0.22
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	9	0.22	0.08	0.22
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	9	0.22	0.08	0.22
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	9	0.2	0.05	0.19
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	9	0.2	0.05	0.19
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	9	0.2	0.05	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	9	0.18	0.08	0.17
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	9	0.18	0.08	0.17
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	9	0.18	0.08	0.17
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	9	0.17	0.05	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	9	0.17	0.05	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	9	0.17	0.05	0.15
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	9	0.17	0.06	0.16
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	9	0.17	0.06	0.16
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	9	0.17	0.06	0.16
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	9	0.16	0.04	0.16
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	9	0.16	0.04	0.16
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	9	0.16	0.04	0.16
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	9	0.16	0.04	0.16
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	9	0.16	0.04	0.16
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	9	0.16	0.04	0.16
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	8	0.29	0.09	0.3
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	8	0.26	0.07	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	8	0.26	0.07	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	8	0.26	0.07	0.26
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	8	0.23	0.1	0.22
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	8	0.23	0.1	0.22
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	8	0.23	0.1	0.22
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	8	0.23	0.07	0.21
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	8	0.23	0.07	0.21
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	8	0.23	0.07	0.21
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	8	0.22	0.06	0.21
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	8	0.22	0.06	0.21
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	8	0.22	0.06	0.21
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	8	0.17	0.04	0.18
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	8	0.17	0.04	0.18
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	8	0.17	0.04	0.18
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	8	0.17	0.08	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	8	0.17	0.08	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	8	0.17	0.08	0.15
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	7	0.26	0.1	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	7	0.26	0.1	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	7	0.26	0.1	0.25
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	7	0.25	0.08	0.26
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	7	0.25	0.08	0.26
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	7	0.25	0.08	0.26
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	7	0.24	0.09	0.25
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	7	0.24	0.09	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	7	0.24	0.09	0.25
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	7	0.24	0.08	0.27
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	7	0.24	0.08	0.27
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	7	0.22	0.08	0.21
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	7	0.22	0.08	0.21
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	7	0.22	0.08	0.21
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	7	0.21	0.04	0.21
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	7	0.21	0.04	0.21
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	7	0.2	0.11	0.16
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	7	0.2	0.11	0.16
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	7	0.2	0.11	0.16
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	7	0.2	0.11	0.16
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	7	0.2	0.11	0.16
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	7	0.2	0.11	0.16
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	7	0.18	0.04	0.19
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	7	0.18	0.04	0.19
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	7	0.18	0.04	0.19
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	7	0.18	0.08	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	7	0.18	0.08	0.14
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	7	0.18	0.05	0.16
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	7	0.18	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	7	0.18	0.05	0.16
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	7	0.18	0.05	0.16
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	7	0.18	0.05	0.16
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	7	0.18	0.05	0.16
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	7	0.18	0.05	0.16
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	7	0.18	0.05	0.16
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	7	0.18	0.05	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	7	0.17	0.04	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	7	0.17	0.04	0.16
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	7	0.16	0.03	0.16
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	7	0.16	0.03	0.16
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	7	0.16	0.03	0.16
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	7	0.16	0.03	0.15
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	7	0.15	0.03	0.16
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	7	0.15	0.03	0.16
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	7	0.15	0.03	0.16
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG12	6	0.35	0.04	0.36
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG13	6	0.35	0.04	0.36
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG21	6	0.29	0.18	0.18
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG22	6	0.29	0.18	0.18
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG23	6	0.29	0.18	0.18
(1,79)	1:137:A:GLY:H	1:138:A:PHE:H	6	0.26	0.11	0.22
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG11	6	0.25	0.09	0.22
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG12	6	0.25	0.09	0.22
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG13	6	0.25	0.09	0.22
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG11	6	0.23	0.1	0.18
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG12	6	0.23	0.1	0.18
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG13	6	0.23	0.1	0.18
(1,247)	1:35:A:ASN:H	1:38:A:TYR:H	6	0.22	0.06	0.22
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG21	6	0.21	0.06	0.22
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG22	6	0.21	0.06	0.22
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG23	6	0.21	0.06	0.22
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG11	6	0.19	0.05	0.19
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG12	6	0.19	0.05	0.19
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG13	6	0.19	0.05	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD11	6	0.19	0.06	0.18
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD12	6	0.19	0.06	0.18
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD13	6	0.19	0.06	0.18
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG21	6	0.17	0.06	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG22	6	0.17	0.06	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG23	6	0.17	0.06	0.15
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD11	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD12	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD13	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD11	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD12	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD13	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD11	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD12	6	0.16	0.04	0.15
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD13	6	0.16	0.04	0.15
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	6	0.16	0.03	0.15
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	6	0.16	0.03	0.15
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD21	6	0.16	0.06	0.12
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD22	6	0.16	0.06	0.12
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD23	6	0.16	0.06	0.12
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE1	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE2	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE3	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE1	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE2	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE3	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE1	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE2	6	0.15	0.03	0.15
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE3	6	0.15	0.03	0.15
(1,242)	1:223:A:GLU:H	1:225:A:GLU:H	6	0.15	0.05	0.14
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB1	6	0.14	0.02	0.14
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB2	6	0.14	0.02	0.14
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB3	6	0.14	0.02	0.14
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG21	6	0.13	0.01	0.13
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG22	6	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG23	6	0.13	0.01	0.13
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	6	0.13	0.02	0.12
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	6	0.13	0.02	0.12
(1,374)	1:225:A:GLU:H	1:230:A:VAL:H	5	0.28	0.13	0.24
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG21	5	0.26	0.07	0.23
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG22	5	0.26	0.07	0.23
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG23	5	0.26	0.07	0.23
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	5	0.25	0.04	0.27
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	5	0.24	0.07	0.27
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	5	0.24	0.07	0.27
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD11	5	0.24	0.14	0.18
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD12	5	0.24	0.14	0.18
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD13	5	0.24	0.14	0.18
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	5	0.24	0.06	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	5	0.24	0.06	0.2
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD21	5	0.23	0.12	0.15
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD22	5	0.23	0.12	0.15
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD23	5	0.23	0.12	0.15
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD11	5	0.22	0.04	0.22
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD12	5	0.22	0.04	0.22
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD13	5	0.22	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,243)	1:224:A:LYS:H	1:226:A:ARG:H	5	0.21	0.17	0.14
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG21	5	0.2	0.1	0.16
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG22	5	0.2	0.1	0.16
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG23	5	0.2	0.1	0.16
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE1	5	0.2	0.08	0.2
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE2	5	0.2	0.08	0.2
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE3	5	0.2	0.08	0.2
(1,341)	1:95:A:GLY:H	1:184:A:THR:H	5	0.19	0.08	0.17
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG21	5	0.19	0.05	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG22	5	0.19	0.05	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG23	5	0.19	0.05	0.15
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG21	5	0.19	0.04	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG22	5	0.19	0.04	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG23	5	0.19	0.04	0.18
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG11	5	0.18	0.08	0.16
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG12	5	0.18	0.08	0.16
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG13	5	0.18	0.08	0.16
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG11	5	0.18	0.07	0.15
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG12	5	0.18	0.07	0.15
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG13	5	0.18	0.07	0.15
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	5	0.17	0.1	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	5	0.17	0.1	0.13
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD11	5	0.17	0.04	0.19
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD12	5	0.17	0.04	0.19
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD13	5	0.17	0.04	0.19
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD21	5	0.16	0.06	0.14
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD22	5	0.16	0.06	0.14
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD23	5	0.16	0.06	0.14
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	5	0.16	0.03	0.15
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	5	0.16	0.03	0.15
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	5	0.16	0.03	0.15
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	5	0.16	0.03	0.15
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	5	0.16	0.03	0.15
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	5	0.16	0.03	0.15
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	5	0.16	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	5	0.16	0.03	0.15
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	5	0.16	0.03	0.15
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	5	0.16	0.02	0.15
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	5	0.16	0.02	0.15
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	5	0.15	0.03	0.15
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD11	5	0.15	0.04	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD12	5	0.15	0.04	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD13	5	0.15	0.04	0.13
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD11	5	0.14	0.03	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD12	5	0.14	0.03	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD13	5	0.14	0.03	0.15
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG21	5	0.14	0.03	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG22	5	0.14	0.03	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG23	5	0.14	0.03	0.13
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD21	5	0.14	0.01	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD22	5	0.14	0.01	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD23	5	0.14	0.01	0.14
(1,57)	1:96:A:ILE:H	1:97:A:GLY:H	4	0.36	0.3	0.2
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	4	0.29	0.14	0.28
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	4	0.29	0.14	0.28
(1,11)	1:41:A:LYS:H	1:42:A:GLU:H	4	0.27	0.1	0.26
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD21	4	0.25	0.03	0.26
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD22	4	0.25	0.03	0.26
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD23	4	0.25	0.03	0.26
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD21	4	0.25	0.03	0.26
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD22	4	0.25	0.03	0.26
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD23	4	0.25	0.03	0.26
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD21	4	0.25	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD22	4	0.25	0.03	0.26
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD23	4	0.25	0.03	0.26
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD11	4	0.24	0.07	0.24
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD12	4	0.24	0.07	0.24
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD13	4	0.24	0.07	0.24
(1,340)	1:93:A:ASP:H	1:186:A:VAL:H	4	0.24	0.07	0.25
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	4	0.24	0.02	0.24
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	4	0.24	0.02	0.24
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD11	4	0.23	0.02	0.24
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD12	4	0.23	0.02	0.24
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD13	4	0.23	0.02	0.24
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG21	4	0.22	0.07	0.2
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG22	4	0.22	0.07	0.2
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG23	4	0.22	0.07	0.2
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG21	4	0.2	0.07	0.18
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG22	4	0.2	0.07	0.18
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG23	4	0.2	0.07	0.18
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD21	4	0.2	0.04	0.2
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD22	4	0.2	0.04	0.2
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD23	4	0.2	0.04	0.2
(1,342)	1:103:A:LEU:H	1:107:A:LEU:H	4	0.2	0.07	0.2
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD11	4	0.19	0.03	0.19
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD12	4	0.19	0.03	0.19
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD13	4	0.19	0.03	0.19
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG21	4	0.19	0.04	0.2
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG22	4	0.19	0.04	0.2
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG23	4	0.19	0.04	0.2
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	4	0.18	0.04	0.18
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	4	0.18	0.04	0.18
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	4	0.18	0.04	0.18
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	4	0.18	0.04	0.18
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	4	0.18	0.04	0.18
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	4	0.18	0.04	0.18
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	4	0.18	0.04	0.18
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	4	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	4	0.18	0.04	0.18
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB1	4	0.17	0.03	0.16
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB2	4	0.17	0.03	0.16
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB3	4	0.17	0.03	0.16
(1,702)	1:31:A:SER:H	1:30:A:MET:HE1	4	0.17	0.08	0.14
(1,702)	1:31:A:SER:H	1:30:A:MET:HE2	4	0.17	0.08	0.14
(1,702)	1:31:A:SER:H	1:30:A:MET:HE3	4	0.17	0.08	0.14
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD11	4	0.17	0.06	0.15
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD12	4	0.17	0.06	0.15
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD13	4	0.17	0.06	0.15
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG21	4	0.17	0.03	0.16
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG22	4	0.17	0.03	0.16
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG23	4	0.17	0.03	0.16
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB1	4	0.17	0.06	0.15
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB2	4	0.17	0.06	0.15
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB3	4	0.17	0.06	0.15
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	4	0.16	0.04	0.17
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	4	0.16	0.04	0.17
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG21	4	0.16	0.04	0.16
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG22	4	0.16	0.04	0.16
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG23	4	0.16	0.04	0.16
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD11	4	0.16	0.02	0.16
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD12	4	0.16	0.02	0.16
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD13	4	0.16	0.02	0.16
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	4	0.16	0.03	0.16
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	4	0.16	0.03	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG11	4	0.16	0.01	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG12	4	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG13	4	0.16	0.01	0.16
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	4	0.16	0.04	0.16
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	4	0.16	0.04	0.16
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	4	0.16	0.02	0.15
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG21	4	0.16	0.04	0.14
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG22	4	0.16	0.04	0.14
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG23	4	0.16	0.04	0.14
(2,80)	1:190:A:LEU:H	1:87:A:ARG:O	4	0.15	0.03	0.14
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG21	4	0.15	0.03	0.15
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG22	4	0.15	0.03	0.15
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG23	4	0.15	0.03	0.15
(1,63)	1:105:A:ASN:H	1:106:A:ASN:H	4	0.15	0.01	0.15
(1,217)	1:180:A:MET:H	1:182:A:ARG:H	4	0.15	0.04	0.14
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG21	4	0.14	0.03	0.14
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG22	4	0.14	0.03	0.14
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG23	4	0.14	0.03	0.14
(1,353)	1:149:A:THR:H	1:187:A:ILE:H	4	0.14	0.03	0.13
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD11	4	0.14	0.01	0.14
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD12	4	0.14	0.01	0.14
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD13	4	0.14	0.01	0.14
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG21	4	0.14	0.02	0.14
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG22	4	0.14	0.02	0.14
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG23	4	0.14	0.02	0.14
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG11	4	0.14	0.03	0.14
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG12	4	0.14	0.03	0.14
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG13	4	0.14	0.03	0.14
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG21	4	0.14	0.04	0.13
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG22	4	0.14	0.04	0.13
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG23	4	0.14	0.04	0.13
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB1	4	0.14	0.03	0.12
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB2	4	0.14	0.03	0.12
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB3	4	0.14	0.03	0.12
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	4	0.13	0.01	0.13
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	4	0.13	0.01	0.13
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	4	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	4	0.13	0.01	0.13
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	4	0.13	0.01	0.13
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	4	0.13	0.01	0.13
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	4	0.13	0.01	0.13
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	4	0.13	0.01	0.13
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	4	0.13	0.01	0.13
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG21	4	0.13	0.02	0.12
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG22	4	0.13	0.02	0.12
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG23	4	0.13	0.02	0.12
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB1	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB2	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB3	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB1	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB2	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB3	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB1	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB2	4	0.12	0.01	0.12
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB3	4	0.12	0.01	0.12
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD11	4	0.12	0.01	0.12
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD12	4	0.12	0.01	0.12
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD13	4	0.12	0.01	0.12
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD11	3	0.3	0.03	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD12	3	0.3	0.03	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD13	3	0.3	0.03	0.32
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	3	0.29	0.05	0.28
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	3	0.29	0.05	0.28
(1,311)	1:55:A:ALA:H	1:96:A:ILE:H	3	0.28	0.08	0.31
(1,122)	1:195:A:THR:H	1:196:A:GLU:H	3	0.27	0.06	0.29
(1,184)	1:72:A:SER:H	1:74:A:LYS:H	3	0.27	0.13	0.23
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	3	0.27	0.01	0.27
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	3	0.27	0.01	0.27
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	3	0.27	0.01	0.27
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	3	0.27	0.01	0.27
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	3	0.27	0.01	0.27
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	3	0.27	0.01	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	3	0.27	0.01	0.27
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	3	0.27	0.01	0.27
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	3	0.27	0.01	0.27
(1,40)	1:75:A:GLU:H	1:76:A:LEU:H	3	0.26	0.04	0.26
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	3	0.25	0.05	0.22
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	3	0.25	0.05	0.22
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD11	3	0.25	0.12	0.2
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD12	3	0.25	0.12	0.2
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD13	3	0.25	0.12	0.2
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	3	0.25	0.12	0.23
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	3	0.25	0.12	0.23
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	3	0.25	0.08	0.28
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	3	0.25	0.08	0.28
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB1	3	0.24	0.08	0.24
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB2	3	0.24	0.08	0.24
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB3	3	0.24	0.08	0.24
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	3	0.22	0.05	0.24
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	3	0.22	0.05	0.24
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	3	0.22	0.05	0.24
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	3	0.22	0.05	0.24
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	3	0.22	0.05	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	3	0.22	0.05	0.24
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	3	0.22	0.05	0.24
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	3	0.22	0.05	0.24
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	3	0.22	0.05	0.24
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD11	3	0.22	0.06	0.21
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD12	3	0.22	0.06	0.21
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD13	3	0.22	0.06	0.21
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	3	0.21	0.11	0.15
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	3	0.21	0.11	0.15
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	3	0.21	0.05	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	3	0.21	0.05	0.17
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	3	0.21	0.05	0.21
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	3	0.21	0.05	0.21
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE1	3	0.2	0.05	0.2
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE2	3	0.2	0.05	0.2
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE3	3	0.2	0.05	0.2
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE1	3	0.2	0.05	0.2
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE2	3	0.2	0.05	0.2
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE3	3	0.2	0.05	0.2
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE1	3	0.2	0.05	0.2
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE2	3	0.2	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE3	3	0.2	0.05	0.2
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD11	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD12	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD13	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD11	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD12	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD13	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD11	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD12	3	0.2	0.04	0.19
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD13	3	0.2	0.04	0.19
(1,362)	1:159:A:GLN:H	1:175:A:ASP:H	3	0.19	0.04	0.21
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD11	3	0.19	0.11	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD12	3	0.19	0.11	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD13	3	0.19	0.11	0.11
(1,270)	1:104:A:ILE:H	1:107:A:LEU:H	3	0.19	0.1	0.14
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG21	3	0.19	0.04	0.2
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG22	3	0.19	0.04	0.2
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG23	3	0.19	0.04	0.2
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG21	3	0.18	0.0	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG22	3	0.18	0.0	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG23	3	0.18	0.0	0.18
(1,348)	1:146:A:GLU:H	1:191:A:LYS:H	3	0.18	0.07	0.13
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG21	3	0.18	0.02	0.19
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG22	3	0.18	0.02	0.19
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG23	3	0.18	0.02	0.19
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD21	3	0.18	0.05	0.19
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD22	3	0.18	0.05	0.19
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD23	3	0.18	0.05	0.19
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD21	3	0.18	0.04	0.18
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD22	3	0.18	0.04	0.18
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD23	3	0.18	0.04	0.18
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	3	0.17	0.05	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	3	0.17	0.05	0.14
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD21	3	0.17	0.05	0.2
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD22	3	0.17	0.05	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD23	3	0.17	0.05	0.2
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD21	3	0.17	0.04	0.19
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD22	3	0.17	0.04	0.19
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD23	3	0.17	0.04	0.19
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD11	3	0.17	0.05	0.19
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD12	3	0.17	0.05	0.19
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD13	3	0.17	0.05	0.19
(1,192)	1:104:A:ILE:H	1:106:A:ASN:H	3	0.16	0.02	0.17
(1,262)	1:69:A:LYS:H	1:72:A:SER:H	3	0.16	0.05	0.13
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	3	0.16	0.04	0.15
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	3	0.16	0.04	0.15
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG21	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG22	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG23	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG21	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG22	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG23	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG21	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG22	3	0.16	0.06	0.14
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG23	3	0.16	0.06	0.14
(2,148)	1:210:A:HIS:H	1:206:A:ILE:O	3	0.16	0.02	0.16
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD11	3	0.16	0.02	0.16
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD12	3	0.16	0.02	0.16
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD13	3	0.16	0.02	0.16
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG21	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG22	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG23	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG21	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG22	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG23	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG21	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG22	3	0.15	0.04	0.13
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG23	3	0.15	0.04	0.13
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG11	3	0.15	0.03	0.16
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG12	3	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG13	3	0.15	0.03	0.16
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG11	3	0.15	0.03	0.16
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG12	3	0.15	0.03	0.16
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG13	3	0.15	0.03	0.16
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG11	3	0.15	0.03	0.16
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG12	3	0.15	0.03	0.16
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG13	3	0.15	0.03	0.16
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD11	3	0.15	0.03	0.14
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD12	3	0.15	0.03	0.14
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD13	3	0.15	0.03	0.14
(1,312)	1:56:A:LEU:H	1:96:A:ILE:H	3	0.14	0.02	0.13
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD11	3	0.14	0.03	0.13
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD12	3	0.14	0.03	0.13
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD13	3	0.14	0.03	0.13
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD21	3	0.14	0.01	0.14
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD22	3	0.14	0.01	0.14
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD23	3	0.14	0.01	0.14
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD21	3	0.13	0.03	0.12
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD22	3	0.13	0.03	0.12
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD23	3	0.13	0.03	0.12
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG21	3	0.13	0.02	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG22	3	0.13	0.02	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG23	3	0.13	0.02	0.15
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG21	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG22	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG23	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG21	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG22	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG23	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG21	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG22	3	0.13	0.03	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG23	3	0.13	0.03	0.11
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD11	3	0.13	0.02	0.12
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD12	3	0.13	0.02	0.12
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD13	3	0.13	0.02	0.12
(1,10)	1:38:A:TYR:H	1:39:A:SER:H	3	0.12	0.01	0.13
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG11	3	0.12	0.01	0.12
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG12	3	0.12	0.01	0.12
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG13	3	0.12	0.01	0.12
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG11	3	0.12	0.01	0.13
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG12	3	0.12	0.01	0.13
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG13	3	0.12	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,66)	1:160:A:TYR:H	1:152:A:THR:O	3	0.12	0.02	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB1	3	0.11	0.0	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB2	3	0.11	0.0	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB3	3	0.11	0.0	0.11
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD21	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD22	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD23	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD21	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD22	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD23	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD21	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD22	2	0.5	0.06	0.5
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD23	2	0.5	0.06	0.5
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG11	2	0.46	0.32	0.46
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG12	2	0.46	0.32	0.46
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG13	2	0.46	0.32	0.46
(1,215)	1:164:A:SER:H	1:166:A:ALA:H	2	0.42	0.05	0.42
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD21	2	0.42	0.11	0.42
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD22	2	0.42	0.11	0.42
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD23	2	0.42	0.11	0.42
(1,260)	1:66:A:ASP:H	1:69:A:LYS:H	2	0.38	0.22	0.38
(1,181)	1:69:A:LYS:H	1:71:A:ASP:H	2	0.37	0.08	0.37
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD21	2	0.34	0.03	0.34
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD22	2	0.34	0.03	0.34
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD23	2	0.34	0.03	0.34
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD11	2	0.32	0.2	0.32
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD12	2	0.32	0.2	0.32
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD13	2	0.32	0.2	0.32
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD21	2	0.3	0.11	0.3
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD22	2	0.3	0.11	0.3
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD23	2	0.3	0.11	0.3
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD11	2	0.29	0.01	0.29
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD12	2	0.29	0.01	0.29
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD13	2	0.29	0.01	0.29
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG21	2	0.28	0.04	0.28
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG22	2	0.28	0.04	0.28
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG23	2	0.28	0.04	0.28
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB1	2	0.27	0.02	0.27
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB2	2	0.27	0.02	0.27
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB3	2	0.27	0.02	0.27
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG21	2	0.26	0.01	0.26
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG22	2	0.26	0.01	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG23	2	0.26	0.01	0.26
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB1	2	0.26	0.02	0.26
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB2	2	0.26	0.02	0.26
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB3	2	0.26	0.02	0.26
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG21	2	0.26	0.02	0.26
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG22	2	0.26	0.02	0.26
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG23	2	0.26	0.02	0.26
(1,139)	1:212:A:GLN:H	1:213:A:PHE:H	2	0.26	0.03	0.26
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	2	0.26	0.05	0.26
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	2	0.26	0.05	0.26
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE1	2	0.26	0.02	0.26
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE2	2	0.26	0.02	0.26
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE3	2	0.26	0.02	0.26
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	2	0.25	0.09	0.25
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	2	0.25	0.09	0.25
(1,288)	1:196:A:GLU:H	1:199:A:GLU:H	2	0.24	0.03	0.24
(1,314)	1:58:A:LYS:H	1:96:A:ILE:H	2	0.24	0.06	0.24
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD11	2	0.23	0.05	0.23
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD12	2	0.23	0.05	0.23
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD13	2	0.23	0.05	0.23
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	2	0.23	0.06	0.23
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	2	0.23	0.06	0.23
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	2	0.23	0.06	0.23
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	2	0.23	0.06	0.23
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	2	0.23	0.06	0.23
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	2	0.23	0.06	0.23
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	2	0.23	0.06	0.23
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	2	0.23	0.06	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	2	0.23	0.06	0.23
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	2	0.22	0.02	0.22
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG21	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG22	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG23	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG21	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG22	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG23	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG21	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG22	2	0.22	0.01	0.22
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG23	2	0.22	0.01	0.22
(1,80)	1:138:A:PHE:H	1:139:A:TYR:H	2	0.22	0.1	0.22
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD11	2	0.22	0.02	0.22
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD12	2	0.22	0.02	0.22
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD13	2	0.22	0.02	0.22
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD11	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD12	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD13	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD11	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD12	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD13	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD11	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD12	2	0.22	0.06	0.22
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD13	2	0.22	0.06	0.22
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD21	2	0.22	0.02	0.22
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD22	2	0.22	0.02	0.22
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD23	2	0.22	0.02	0.22
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	2	0.22	0.04	0.22
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	2	0.22	0.04	0.22
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD21	2	0.22	0.04	0.22
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD22	2	0.22	0.04	0.22
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD23	2	0.22	0.04	0.22
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD11	2	0.21	0.01	0.21
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD12	2	0.21	0.01	0.21
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD13	2	0.21	0.01	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,153)	1:24:A:ALA:H	1:26:A:ILE:H	2	0.21	0.1	0.21
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG21	2	0.2	0.0	0.2
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG22	2	0.2	0.0	0.2
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG23	2	0.2	0.0	0.2
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD11	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD12	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD13	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD11	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD12	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD13	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD11	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD12	2	0.2	0.05	0.2
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD13	2	0.2	0.05	0.2
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD11	2	0.2	0.01	0.2
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD12	2	0.2	0.01	0.2
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD13	2	0.2	0.01	0.2
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB1	2	0.2	0.09	0.2
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB2	2	0.2	0.09	0.2
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB3	2	0.2	0.09	0.2
(1,41)	1:76:A:LEU:H	1:77:A:HIS:H	2	0.2	0.08	0.2
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG21	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG22	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG23	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG21	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG22	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG23	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG21	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG22	2	0.2	0.01	0.2
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG23	2	0.2	0.01	0.2
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD21	2	0.2	0.09	0.2
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD22	2	0.2	0.09	0.2
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD23	2	0.2	0.09	0.2
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG21	2	0.2	0.09	0.2
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG22	2	0.2	0.09	0.2
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG23	2	0.2	0.09	0.2
(1,208)	1:136:A:VAL:H	1:138:A:PHE:H	2	0.19	0.02	0.19
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG11	2	0.19	0.04	0.19
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG12	2	0.19	0.04	0.19
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG13	2	0.19	0.04	0.19
(1,267)	1:99:A:THR:H	1:102:A:ASP:H	2	0.18	0.04	0.18
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG21	2	0.18	0.08	0.18
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG22	2	0.18	0.08	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG23	2	0.18	0.08	0.18
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG21	2	0.18	0.08	0.18
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG22	2	0.18	0.08	0.18
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG23	2	0.18	0.08	0.18
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG21	2	0.18	0.02	0.18
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG22	2	0.18	0.02	0.18
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG23	2	0.18	0.02	0.18
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG11	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG12	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG13	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG11	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG12	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG13	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG11	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG12	2	0.18	0.05	0.18
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG13	2	0.18	0.05	0.18
(1,101)	1:168:A:GLY:H	1:169:A:SER:H	2	0.18	0.06	0.18
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD11	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD12	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD13	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD11	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD12	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD13	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD11	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD12	2	0.18	0.04	0.18
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD13	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	2	0.18	0.04	0.18
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	2	0.18	0.04	0.18
(1,107)	1:176:A:THR:H	1:177:A:GLY:H	2	0.17	0.0	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE1	2	0.17	0.0	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE2	2	0.17	0.0	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE3	2	0.17	0.0	0.17
(1,282)	1:138:A:PHE:H	1:141:A:ALA:H	2	0.17	0.02	0.17
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD21	2	0.17	0.05	0.17
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD22	2	0.17	0.05	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD23	2	0.17	0.05	0.17
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD11	2	0.16	0.02	0.16
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD12	2	0.16	0.02	0.16
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD13	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG21	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG22	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG23	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG21	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG22	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG23	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG21	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG22	2	0.16	0.02	0.16
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG23	2	0.16	0.02	0.16
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG21	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG22	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG23	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG21	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG22	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG23	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG21	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG22	2	0.16	0.01	0.16
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG23	2	0.16	0.01	0.16
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG21	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG22	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG23	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG21	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG22	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG23	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG21	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG22	2	0.16	0.02	0.16
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG23	2	0.16	0.02	0.16
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD11	2	0.16	0.01	0.16
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD12	2	0.16	0.01	0.16
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD13	2	0.16	0.01	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG21	2	0.16	0.0	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG22	2	0.16	0.0	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG23	2	0.16	0.0	0.16
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG21	2	0.16	0.06	0.16
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG22	2	0.16	0.06	0.16
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG23	2	0.16	0.06	0.16
(1,180)	1:68:A:SER:H	1:70:A:LEU:H	2	0.16	0.02	0.16
(1,343)	1:114:A:GLY:H	1:118:A:PHE:H	2	0.16	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD11	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD12	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD13	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD11	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD12	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD13	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD11	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD12	2	0.16	0.05	0.16
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD13	2	0.16	0.05	0.16
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG21	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG22	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG23	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG21	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG22	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG23	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG21	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG22	2	0.16	0.02	0.16
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG23	2	0.16	0.02	0.16
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	2	0.16	0.01	0.16
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	2	0.16	0.01	0.16
(2,96)	1:35:A:ASN:H	1:31:A:SER:O	2	0.16	0.05	0.16
(2,150)	1:211:A:SER:H	1:207:A:VAL:O	2	0.16	0.05	0.16
(1,73)	1:127:A:ASP:H	1:128:A:ILE:H	2	0.15	0.02	0.15
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD21	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD22	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD23	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD21	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD22	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD23	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD21	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD22	2	0.15	0.01	0.15
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD23	2	0.15	0.01	0.15
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD11	2	0.15	0.02	0.15
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD12	2	0.15	0.02	0.15
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD13	2	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG11	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG12	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG13	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG11	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG12	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG13	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG11	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG12	2	0.15	0.03	0.15
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG13	2	0.15	0.03	0.15
(1,182)	1:70:A:LEU:H	1:72:A:SER:H	2	0.15	0.03	0.15
(1,278)	1:131:A:ILE:H	1:134:A:PHE:H	2	0.15	0.03	0.15
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD11	2	0.15	0.04	0.15
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD12	2	0.15	0.04	0.15
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD13	2	0.15	0.04	0.15
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG21	2	0.15	0.03	0.15
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG22	2	0.15	0.03	0.15
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG23	2	0.15	0.03	0.15
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG21	2	0.15	0.04	0.15
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG22	2	0.15	0.04	0.15
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG23	2	0.15	0.04	0.15
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	2	0.15	0.0	0.15
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD11	2	0.14	0.03	0.14
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD12	2	0.14	0.03	0.14
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD13	2	0.14	0.03	0.14
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	2	0.14	0.01	0.14
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	2	0.14	0.01	0.14
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD21	2	0.14	0.02	0.14
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD22	2	0.14	0.02	0.14
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD23	2	0.14	0.02	0.14
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG11	2	0.14	0.04	0.14
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG12	2	0.14	0.04	0.14
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG13	2	0.14	0.04	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD11	2	0.14	0.0	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD12	2	0.14	0.0	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD13	2	0.14	0.0	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB1	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB2	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB3	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB1	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB2	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB3	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB1	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB2	2	0.14	0.02	0.14
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB3	2	0.14	0.02	0.14
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD11	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD12	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD13	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD11	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD12	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD13	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD11	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD12	2	0.14	0.04	0.14
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD13	2	0.14	0.04	0.14
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE1	2	0.14	0.02	0.14
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE2	2	0.14	0.02	0.14
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE3	2	0.14	0.02	0.14
(2,30)	1:88:A:THR:H	1:83:A:ASN:O	2	0.14	0.01	0.14
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	2	0.13	0.01	0.13
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	2	0.13	0.01	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG21	2	0.13	0.0	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG22	2	0.13	0.0	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG23	2	0.13	0.0	0.13
(2,12)	1:78:A:ILE:H	1:217:A:PRO:O	2	0.13	0.02	0.13
(2,68)	1:153:A:LYS:H	1:183:A:GLY:O	2	0.13	0.01	0.13
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB1	2	0.12	0.02	0.12
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB2	2	0.12	0.02	0.12
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB3	2	0.12	0.02	0.12
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB1	2	0.12	0.02	0.12
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB2	2	0.12	0.02	0.12
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB3	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)
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB1	2	0.12	0.02	0.12
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB2	2	0.12	0.02	0.12
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB3	2	0.12	0.02	0.12
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD21	2	0.12	0.01	0.12
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD22	2	0.12	0.01	0.12
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD23	2	0.12	0.01	0.12
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD11	2	0.12	0.02	0.12
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD12	2	0.12	0.02	0.12
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD13	2	0.12	0.02	0.12
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG21	2	0.12	0.01	0.12
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG22	2	0.12	0.01	0.12
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG23	2	0.12	0.01	0.12
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG21	2	0.12	0.01	0.12
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG22	2	0.12	0.01	0.12
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG23	2	0.12	0.01	0.12
(2,92)	1:33:A:ILE:H	1:29:A:LEU:O	2	0.12	0.01	0.12
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG21	2	0.12	0.02	0.12
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG22	2	0.12	0.02	0.12
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG23	2	0.12	0.02	0.12
(2,16)	1:79:A:ASN:H	1:92:A:VAL:O	2	0.12	0.02	0.12
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD11	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD12	2	0.12	0.01	0.12
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD13	2	0.12	0.01	0.12
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG21	2	0.12	0.02	0.12
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG22	2	0.12	0.02	0.12
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG23	2	0.12	0.02	0.12
(1,281)	1:136:A:VAL:H	1:139:A:TYR:H	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	2	0.12	0.0	0.12
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	2	0.12	0.0	0.12

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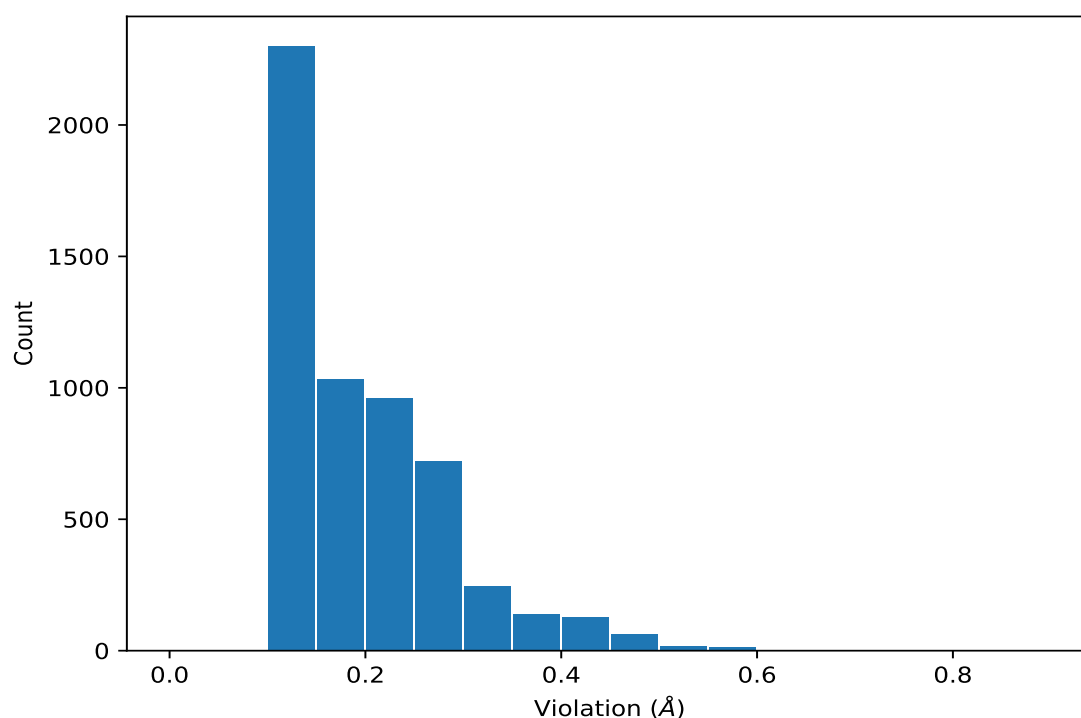
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB1	2	0.12	0.0	0.12
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB2	2	0.12	0.0	0.12
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB3	2	0.12	0.0	0.12
(1,200)	1:123:A:GLN:H	1:125:A:GLY:H	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD11	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD12	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD13	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD11	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD12	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD13	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD11	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD12	2	0.11	0.01	0.11
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD13	2	0.11	0.01	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG11	2	0.11	0.0	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG12	2	0.11	0.0	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG13	2	0.11	0.0	0.11
(1,35)	1:69:A:LYS:H	1:70:A:LEU:H	2	0.11	0.0	0.11
(1,337)	1:89:A:LEU:H	1:190:A:LEU:H	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG11	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG12	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG13	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG11	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG12	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG13	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG11	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG12	2	0.11	0.0	0.11
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG13	2	0.11	0.0	0.11
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG21	2	0.1	0.0	0.1
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG22	2	0.1	0.0	0.1
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG23	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)
(1,57)	1:96:A:ILE:H	1:97:A:GLY:H	8	0.88
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG11	2	0.79
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG12	2	0.79
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG13	2	0.79
(1,260)	1:66:A:ASP:H	1:69:A:LYS:H	8	0.61
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG21	5	0.57
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG22	5	0.57
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG23	5	0.57
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD21	3	0.57
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD22	3	0.57
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD23	3	0.57
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD21	3	0.57
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD22	3	0.57
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD23	3	0.57
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD21	3	0.57
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD22	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD23	3	0.57
(1,243)	1:224:A:LYS:H	1:226:A:ARG:H	7	0.55
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	8	0.54
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	8	0.54
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	8	0.54
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	8	0.54
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	8	0.54
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	8	0.54
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	8	0.54
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	8	0.54
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	8	0.54
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG21	9	0.52
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG22	9	0.52
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG23	9	0.52
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD21	3	0.52
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD22	3	0.52
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD23	3	0.52
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD11	6	0.51
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD12	6	0.51
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD13	6	0.51
(1,79)	1:137:A:GLY:H	1:138:A:PHE:H	2	0.5
(1,264)	1:83:A:ASN:H	1:86:A:ASP:H	5	0.49
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	3	0.48
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	3	0.48
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	3	0.48
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	3	0.48
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	3	0.48
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	3	0.48
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	3	0.48
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	3	0.48
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	3	0.48
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD11	2	0.47
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD12	2	0.47
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD13	2	0.47
(1,823)	1:89:A:LEU:H	1:88:A:THR:HG21	5	0.47
(1,823)	1:89:A:LEU:H	1:88:A:THR:HG22	5	0.47
(1,823)	1:89:A:LEU:H	1:88:A:THR:HG23	5	0.47
(1,215)	1:164:A:SER:H	1:166:A:ALA:H	1	0.47
(1,977)	1:172:A:VAL:H	1:171:A:THR:HG21	7	0.46
(1,977)	1:172:A:VAL:H	1:171:A:THR:HG22	7	0.46
(1,977)	1:172:A:VAL:H	1:171:A:THR:HG23	7	0.46
(1,955)	1:161:A:ALA:H	1:172:A:VAL:HG11	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:161:A:ALA:H	1:172:A:VAL:HG12	5	0.46
(1,955)	1:161:A:ALA:H	1:172:A:VAL:HG13	5	0.46
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	9	0.46
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	9	0.46
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	9	0.46
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	1	0.46
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	1	0.46
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	1	0.46
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	1	0.46
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	1	0.46
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	1	0.46
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	1	0.46
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	1	0.46
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	1	0.46
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	7	0.45
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	7	0.45
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	7	0.45
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	2	0.45
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	2	0.45
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	2	0.45
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	6	0.45
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	6	0.45
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	6	0.45
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	6	0.45
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	6	0.45
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	6	0.45
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	6	0.45
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	6	0.45
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	6	0.45
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	4	0.45
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	4	0.45
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	4	0.45
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	4	0.45
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	4	0.45
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	4	0.45
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	4	0.45
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	4	0.45
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	4	0.45
(1,374)	1:225:A:GLU:H	1:230:A:VAL:H	3	0.45
(1,184)	1:72:A:SER:H	1:74:A:LYS:H	4	0.45
(1,181)	1:69:A:LYS:H	1:71:A:ASP:H	9	0.45
(1,994)	1:185:A:LYS:H	1:150:A:VAL:HG21	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:185:A:LYS:H	1:150:A:VAL:HG22	2	0.44
(1,994)	1:185:A:LYS:H	1:150:A:VAL:HG23	2	0.44
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	8	0.44
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	8	0.44
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	8	0.44
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	8	0.44
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	8	0.44
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	8	0.44
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	8	0.44
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	8	0.44
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	8	0.44
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD21	9	0.44
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD22	9	0.44
(1,483)	1:59:A:ILE:HD11	1:70:A:LEU:HD23	9	0.44
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD21	9	0.44
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD22	9	0.44
(1,483)	1:59:A:ILE:HD12	1:70:A:LEU:HD23	9	0.44
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD21	9	0.44
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD22	9	0.44
(1,483)	1:59:A:ILE:HD13	1:70:A:LEU:HD23	9	0.44
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	10	0.43
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	10	0.43
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	10	0.43
(1,860)	1:107:A:LEU:H	1:109:A:THR:HG21	4	0.43
(1,860)	1:107:A:LEU:H	1:109:A:THR:HG22	4	0.43
(1,860)	1:107:A:LEU:H	1:109:A:THR:HG23	4	0.43
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	5	0.43
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	5	0.43
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	5	0.43
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	5	0.43
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	5	0.43
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	5	0.43
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	5	0.43
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	5	0.43
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	5	0.43
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG11	4	0.42
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG12	4	0.42
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG13	4	0.42
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD11	6	0.42
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD12	6	0.42
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD13	6	0.42
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG11	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG12	3	0.42
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG13	3	0.42
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	1	0.42
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	1	0.42
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	1	0.42
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	1	0.42
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	1	0.42
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	1	0.42
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	1	0.42
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	1	0.42
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	1	0.42
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	7	0.42
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	7	0.42
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	7	0.42
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	7	0.42
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	7	0.42
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	7	0.42
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	7	0.42
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	7	0.42
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	7	0.42
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	6	0.41
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	6	0.41
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	6	0.41
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	1	0.41
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	1	0.41
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	1	0.41
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	1	0.41
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	1	0.41
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	1	0.41
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	1	0.41
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	1	0.41
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	1	0.41
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	4	0.41
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	4	0.41
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	4	0.41
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	4	0.41
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	4	0.41
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	4	0.41
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	4	0.41
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	4	0.41
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	4	0.41
(1,374)	1:225:A:GLU:H	1:230:A:VAL:H	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:41:A:LYS:H	1:42:A:GLU:H	2	0.41
(1,981)	1:173:A:ARG:H	1:172:A:VAL:HG11	5	0.4
(1,981)	1:173:A:ARG:H	1:172:A:VAL:HG12	5	0.4
(1,981)	1:173:A:ARG:H	1:172:A:VAL:HG13	5	0.4
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG21	9	0.4
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG22	9	0.4
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG23	9	0.4
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD21	4	0.4
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD22	4	0.4
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD23	4	0.4
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	2	0.4
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	2	0.4
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	2	0.4
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG12	4	0.4
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG13	4	0.4
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	2	0.4
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	2	0.4
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	2	0.4
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	2	0.4
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	2	0.4
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	2	0.4
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	2	0.4
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	2	0.4
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	2	0.4
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	2	0.4
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	2	0.4
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	2	0.4
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	2	0.4
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	2	0.4
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	2	0.4
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	2	0.4
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	2	0.4
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	2	0.4
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	4	0.4
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	4	0.4
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	4	0.4
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	4	0.4
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	4	0.4
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	4	0.4
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	4	0.4
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	4	0.4
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	4	0.4
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	5	0.39
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	5	0.39
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	5	0.39
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	3	0.39
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	3	0.39
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	3	0.39
(1,772)	1:69:A:LYS:H	1:70:A:LEU:HD11	4	0.39
(1,772)	1:69:A:LYS:H	1:70:A:LEU:HD12	4	0.39
(1,772)	1:69:A:LYS:H	1:70:A:LEU:HD13	4	0.39
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	4	0.39
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	4	0.39
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	4	0.39
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	4	0.39
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	4	0.39
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	4	0.39
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	4	0.39
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	4	0.39
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	4	0.39
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	8	0.39
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	7	0.38
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	7	0.38
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	7	0.38
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	5	0.38
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	5	0.38
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	5	0.38
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	2	0.38
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	2	0.38
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	2	0.38
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	3	0.38
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	3	0.38
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	3	0.38
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD21	6	0.38
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD22	6	0.38
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD23	6	0.38
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG12	9	0.38
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG13	9	0.38
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG21	9	0.37
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG22	9	0.37
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG23	9	0.37
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	2	0.37
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	2	0.37
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD21	1	0.37
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD22	1	0.37
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD23	1	0.37
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	9	0.37
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	9	0.37
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	9	0.37
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD21	3	0.37
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD22	3	0.37
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD23	3	0.37
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG12	6	0.37
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG13	6	0.37
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	3	0.37
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	3	0.37
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	3	0.37
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	3	0.37
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	3	0.37
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	3	0.37
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	3	0.37
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	3	0.37
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	3	0.37
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	5	0.37
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	5	0.37
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	5	0.37
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	5	0.37
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	5	0.37
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	5	0.37
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	5	0.37
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	5	0.37
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	5	0.37
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	10	0.37
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	10	0.37
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	10	0.37
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	10	0.37
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	10	0.37
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	10	0.37
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	10	0.37
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	10	0.37
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	10	0.37
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	8	0.37
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	8	0.37
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	8	0.37
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	8	0.37
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	8	0.37
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	8	0.37
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	8	0.37
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	8	0.37
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	6	0.37
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	6	0.37
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	6	0.37
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	6	0.37
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	6	0.37
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	6	0.37
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	6	0.37
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	6	0.37
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	6	0.37
(1,215)	1:164:A:SER:H	1:166:A:ALA:H	2	0.37
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	9	0.36
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	9	0.36
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	9	0.36
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	10	0.36
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	10	0.36
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	10	0.36
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	10	0.36
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	10	0.36
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	10	0.36
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	10	0.36
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	10	0.36
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	10	0.36
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	1	0.36
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	1	0.36
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	1	0.36
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	1	0.36
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	1	0.36
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	1	0.36
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	1	0.36
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	1	0.36
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	1	0.36
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	9	0.36
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	9	0.36
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	9	0.36
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	9	0.36
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	9	0.36
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	9	0.36
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	9	0.36
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	9	0.36
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	8	0.36
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	8	0.36
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	8	0.36
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	8	0.36
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	8	0.36
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	8	0.36
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	8	0.36
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	8	0.36
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	8	0.36
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	2	0.36
(1,933)	1:149:A:THR:H	1:150:A:VAL:HG11	2	0.35
(1,933)	1:149:A:THR:H	1:150:A:VAL:HG12	2	0.35
(1,933)	1:149:A:THR:H	1:150:A:VAL:HG13	2	0.35
(1,813)	1:84:A:LYS:H	1:198:A:LEU:HD11	5	0.35
(1,813)	1:84:A:LYS:H	1:198:A:LEU:HD12	5	0.35
(1,813)	1:84:A:LYS:H	1:198:A:LEU:HD13	5	0.35
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	1	0.35
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	1	0.35
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	1	0.35
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD11	3	0.35
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD12	3	0.35
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD13	3	0.35
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG12	2	0.35
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG13	2	0.35
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	7	0.35
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	7	0.35
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	7	0.35
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	7	0.35
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	7	0.35
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	7	0.35
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	7	0.35
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	7	0.35
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	7	0.35
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	3	0.35
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	3	0.35
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	3	0.35
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	3	0.35
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	3	0.35
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	3	0.35
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	3	0.35
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	3	0.35
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	4	0.35
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	4	0.35
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	4	0.35
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	4	0.35
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	4	0.35
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	4	0.35
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	4	0.35
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	4	0.35
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	4	0.35
(1,434)	1:32:A:LEU:HD21	1:122:A:LEU:HD21	8	0.35
(1,434)	1:32:A:LEU:HD21	1:122:A:LEU:HD22	8	0.35
(1,434)	1:32:A:LEU:HD21	1:122:A:LEU:HD23	8	0.35
(1,434)	1:32:A:LEU:HD22	1:122:A:LEU:HD21	8	0.35
(1,434)	1:32:A:LEU:HD22	1:122:A:LEU:HD22	8	0.35
(1,434)	1:32:A:LEU:HD22	1:122:A:LEU:HD23	8	0.35
(1,434)	1:32:A:LEU:HD23	1:122:A:LEU:HD21	8	0.35
(1,434)	1:32:A:LEU:HD23	1:122:A:LEU:HD22	8	0.35
(1,434)	1:32:A:LEU:HD23	1:122:A:LEU:HD23	8	0.35
(1,311)	1:55:A:ALA:H	1:96:A:ILE:H	6	0.35
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	9	0.34
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	9	0.34
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	9	0.34
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD11	3	0.34
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD12	3	0.34
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD13	3	0.34
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB1	3	0.34
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB2	3	0.34
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB3	3	0.34
(1,818)	1:86:A:ASP:H	1:198:A:LEU:HD11	5	0.34
(1,818)	1:86:A:ASP:H	1:198:A:LEU:HD12	5	0.34
(1,818)	1:86:A:ASP:H	1:198:A:LEU:HD13	5	0.34
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	8	0.34
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	8	0.34
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	8	0.34
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	8	0.34
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	8	0.34
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	8	0.34
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	8	0.34
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	8	0.34
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	5	0.34
(1,340)	1:93:A:ASP:H	1:186:A:VAL:H	2	0.34
(1,265)	1:84:A:LYS:H	1:87:A:ARG:H	5	0.34
(1,122)	1:195:A:THR:H	1:196:A:GLU:H	4	0.34
(1,94)	1:158:A:GLU:H	1:159:A:GLN:H	7	0.34
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE1	8	0.33
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE2	8	0.33
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE3	8	0.33
(1,821)	1:87:A:ARG:H	1:198:A:LEU:HD11	8	0.33
(1,821)	1:87:A:ARG:H	1:198:A:LEU:HD12	8	0.33
(1,821)	1:87:A:ARG:H	1:198:A:LEU:HD13	8	0.33
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	10	0.33
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	10	0.33
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	10	0.33
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG11	8	0.33
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG12	8	0.33
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG13	8	0.33
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	3	0.33
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	3	0.33
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	3	0.33
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	3	0.33
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	3	0.33
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	3	0.33
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	3	0.33
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	3	0.33
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	3	0.33
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	9	0.33
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	9	0.33
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	9	0.33
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	9	0.33
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	9	0.33
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	9	0.33
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	9	0.33
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	9	0.33
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	9	0.33
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	5	0.33
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	5	0.33
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	5	0.33
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	5	0.33
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	5	0.33
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	5	0.33
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	5	0.33
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	5	0.33
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	9	0.33
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	9	0.33
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	9	0.33
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	9	0.33
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	9	0.33
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	9	0.33
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	9	0.33
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	9	0.33
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	9	0.33
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	8	0.33
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	8	0.33
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	8	0.33
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	8	0.33
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	8	0.33
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	8	0.33
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	8	0.33
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	8	0.33
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	8	0.33
(1,1113)	1:225:A:GLU:H	1:222:A:VAL:HG21	9	0.32
(1,1113)	1:225:A:GLU:H	1:222:A:VAL:HG22	9	0.32
(1,1113)	1:225:A:GLU:H	1:222:A:VAL:HG23	9	0.32
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	10	0.32
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	10	0.32
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	10	0.32
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG21	5	0.32
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG22	5	0.32
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG23	5	0.32
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	10	0.32
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	10	0.32
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	10	0.32
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	5	0.32
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	5	0.32
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	5	0.32
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	6	0.32
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	6	0.32
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	6	0.32
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG21	7	0.32
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG22	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG23	7	0.32
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG11	4	0.32
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG12	4	0.32
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG13	4	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD11	2	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD12	2	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD13	2	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD11	7	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD12	7	0.32
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD13	7	0.32
(1,608)	1:17:A:VAL:H	1:17:A:VAL:HG21	2	0.32
(1,608)	1:17:A:VAL:H	1:17:A:VAL:HG22	2	0.32
(1,608)	1:17:A:VAL:H	1:17:A:VAL:HG23	2	0.32
(1,341)	1:95:A:GLY:H	1:184:A:THR:H	7	0.32
(1,270)	1:104:A:ILE:H	1:107:A:LEU:H	1	0.32
(1,80)	1:138:A:PHE:H	1:139:A:TYR:H	3	0.32
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	1	0.31
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	1	0.31
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	1	0.31
(1,957)	1:162:A:TRP:H	1:103:A:LEU:HD11	1	0.31
(1,957)	1:162:A:TRP:H	1:103:A:LEU:HD12	1	0.31
(1,957)	1:162:A:TRP:H	1:103:A:LEU:HD13	1	0.31
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG21	10	0.31
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG22	10	0.31
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG23	10	0.31
(1,937)	1:150:A:VAL:H	1:151:A:ILE:HD11	3	0.31
(1,937)	1:150:A:VAL:H	1:151:A:ILE:HD12	3	0.31
(1,937)	1:150:A:VAL:H	1:151:A:ILE:HD13	3	0.31
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	3	0.31
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	3	0.31
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	3	0.31
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	7	0.31
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	7	0.31
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	7	0.31
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD21	9	0.31
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD22	9	0.31
(1,776)	1:71:A:ASP:H	1:70:A:LEU:HD23	9	0.31
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD21	6	0.31
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD22	6	0.31
(1,724)	1:44:A:PHE:H	1:143:A:LEU:HD23	6	0.31
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	10	0.31
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	10	0.31
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	7	0.31
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	7	0.31
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	7	0.31
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG21	9	0.31
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG22	9	0.31
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG23	9	0.31
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG12	8	0.31
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG13	8	0.31
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	6	0.31
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	6	0.31
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	6	0.31
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	6	0.31
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	6	0.31
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	6	0.31
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	6	0.31
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	6	0.31
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	6	0.31
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	9	0.31
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	9	0.31
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	9	0.31
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	9	0.31
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	9	0.31
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	9	0.31
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	9	0.31
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	9	0.31
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	9	0.31
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	2	0.31
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	2	0.31
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	2	0.31
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	2	0.31
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	2	0.31
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	2	0.31
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	2	0.31
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	2	0.31
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	2	0.31
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	8	0.31
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	8	0.31
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	8	0.31
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	8	0.31
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	8	0.31
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	8	0.31
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	8	0.31
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	8	0.31
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	4	0.31
(1,311)	1:55:A:ALA:H	1:96:A:ILE:H	8	0.31
(1,247)	1:35:A:ASN:H	1:38:A:TYR:H	2	0.31
(1,153)	1:24:A:ALA:H	1:26:A:ILE:H	10	0.31
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	1	0.3
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	1	0.3
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	1	0.3
(1,972)	1:169:A:SER:H	1:30:A:MET:HE1	3	0.3
(1,972)	1:169:A:SER:H	1:30:A:MET:HE2	3	0.3
(1,972)	1:169:A:SER:H	1:30:A:MET:HE3	3	0.3
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD11	3	0.3
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD12	3	0.3
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD13	3	0.3
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG21	2	0.3
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG22	2	0.3
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG23	2	0.3
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD11	8	0.3
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD12	8	0.3
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD13	8	0.3
(1,808)	1:83:A:ASN:H	1:88:A:THR:HG21	6	0.3
(1,808)	1:83:A:ASN:H	1:88:A:THR:HG22	6	0.3
(1,808)	1:83:A:ASN:H	1:88:A:THR:HG23	6	0.3
(1,773)	1:69:A:LYS:H	1:70:A:LEU:HD21	4	0.3
(1,773)	1:69:A:LYS:H	1:70:A:LEU:HD22	4	0.3
(1,773)	1:69:A:LYS:H	1:70:A:LEU:HD23	4	0.3
(1,702)	1:31:A:SER:H	1:30:A:MET:HE1	5	0.3
(1,702)	1:31:A:SER:H	1:30:A:MET:HE2	5	0.3
(1,702)	1:31:A:SER:H	1:30:A:MET:HE3	5	0.3
(1,642)	1:107:A:LEU:H	1:107:A:LEU:HD11	7	0.3
(1,642)	1:107:A:LEU:H	1:107:A:LEU:HD12	7	0.3
(1,642)	1:107:A:LEU:H	1:107:A:LEU:HD13	7	0.3
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	7	0.3
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	7	0.3
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	7	0.3
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	7	0.3
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	7	0.3
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	7	0.3
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	7	0.3
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	7	0.3
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	1	0.3
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	1	0.3
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	1	0.3
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	1	0.3
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	1	0.3
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	1	0.3
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	1	0.3
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	1	0.3
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	1	0.3
(1,314)	1:58:A:LYS:H	1:96:A:ILE:H	8	0.3
(1,272)	1:117:A:ALA:H	1:120:A:GLU:H	1	0.3
(1,40)	1:75:A:GLU:H	1:76:A:LEU:H	6	0.3
(1,11)	1:41:A:LYS:H	1:42:A:GLU:H	1	0.3
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	8	0.29
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	8	0.29
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	8	0.29
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG21	2	0.29
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG22	2	0.29
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG23	2	0.29
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	6	0.29
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	6	0.29
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	6	0.29
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	2	0.29
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	2	0.29
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	2	0.29
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	10	0.29
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	10	0.29
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	10	0.29
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB1	6	0.29
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB2	6	0.29
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB3	6	0.29
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD11	3	0.29
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD12	3	0.29
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD13	3	0.29
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB1	5	0.29
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB2	5	0.29
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB3	5	0.29
(1,692)	1:26:A:ILE:H	1:24:A:ALA:HB1	9	0.29
(1,692)	1:26:A:ILE:H	1:24:A:ALA:HB2	9	0.29
(1,692)	1:26:A:ILE:H	1:24:A:ALA:HB3	9	0.29
(1,581)	1:150:A:VAL:HG21	1:186:A:VAL:HG11	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:150:A:VAL:HG21	1:186:A:VAL:HG12	2	0.29
(1,581)	1:150:A:VAL:HG21	1:186:A:VAL:HG13	2	0.29
(1,581)	1:150:A:VAL:HG22	1:186:A:VAL:HG11	2	0.29
(1,581)	1:150:A:VAL:HG22	1:186:A:VAL:HG12	2	0.29
(1,581)	1:150:A:VAL:HG22	1:186:A:VAL:HG13	2	0.29
(1,581)	1:150:A:VAL:HG23	1:186:A:VAL:HG11	2	0.29
(1,581)	1:150:A:VAL:HG23	1:186:A:VAL:HG12	2	0.29
(1,581)	1:150:A:VAL:HG23	1:186:A:VAL:HG13	2	0.29
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	6	0.29
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	6	0.29
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	6	0.29
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	6	0.29
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	6	0.29
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	6	0.29
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	6	0.29
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	6	0.29
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	6	0.29
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	2	0.29
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	2	0.29
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	2	0.29
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	2	0.29
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	2	0.29
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	2	0.29
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	2	0.29
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	2	0.29
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	2	0.29
(1,187)	1:85:A:GLN:H	1:87:A:ARG:H	5	0.29
(1,181)	1:69:A:LYS:H	1:71:A:ASP:H	4	0.29
(1,139)	1:212:A:GLN:H	1:213:A:PHE:H	4	0.29
(1,122)	1:195:A:THR:H	1:196:A:GLU:H	6	0.29
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG11	9	0.28
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG12	9	0.28
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG13	9	0.28
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	8	0.28
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	8	0.28
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	8	0.28
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD11	6	0.28
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD12	6	0.28
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD13	6	0.28
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	10	0.28
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	10	0.28
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	6	0.28
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	6	0.28
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	6	0.28
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD21	2	0.28
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD22	2	0.28
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD23	2	0.28
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG21	8	0.28
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG22	8	0.28
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG23	8	0.28
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB1	8	0.28
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB2	8	0.28
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB3	8	0.28
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD21	2	0.28
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD22	2	0.28
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD23	2	0.28
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD11	3	0.28
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD12	3	0.28
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD13	3	0.28
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	4	0.28
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	4	0.28
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	4	0.28
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG11	2	0.28
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG12	2	0.28
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG13	2	0.28
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG12	1	0.28
(1,616)	1:43:A:ILE:H	1:43:A:ILE:HG13	1	0.28
(1,591)	1:188:A:LEU:HD21	1:190:A:LEU:HD21	4	0.28
(1,591)	1:188:A:LEU:HD21	1:190:A:LEU:HD22	4	0.28
(1,591)	1:188:A:LEU:HD21	1:190:A:LEU:HD23	4	0.28
(1,591)	1:188:A:LEU:HD22	1:190:A:LEU:HD21	4	0.28
(1,591)	1:188:A:LEU:HD22	1:190:A:LEU:HD22	4	0.28
(1,591)	1:188:A:LEU:HD22	1:190:A:LEU:HD23	4	0.28
(1,591)	1:188:A:LEU:HD23	1:190:A:LEU:HD21	4	0.28
(1,591)	1:188:A:LEU:HD23	1:190:A:LEU:HD22	4	0.28
(1,591)	1:188:A:LEU:HD23	1:190:A:LEU:HD23	4	0.28
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD21	9	0.28
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD22	9	0.28
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD23	9	0.28
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD21	9	0.28
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD22	9	0.28
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD23	9	0.28
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD21	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD22	9	0.28
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD23	9	0.28
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	4	0.28
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	4	0.28
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	4	0.28
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	4	0.28
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	4	0.28
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	4	0.28
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	4	0.28
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	4	0.28
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	4	0.28
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	3	0.28
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	3	0.28
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	3	0.28
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	3	0.28
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	3	0.28
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	3	0.28
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	3	0.28
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	3	0.28
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	3	0.28
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	4	0.28
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	4	0.28
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	4	0.28
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	4	0.28
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	4	0.28
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	4	0.28
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	4	0.28
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	4	0.28
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	4	0.28
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	8	0.28
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	8	0.28
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	8	0.28
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	8	0.28
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	8	0.28
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	8	0.28
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	8	0.28
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	8	0.28
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	8	0.28
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	8	0.28
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	8	0.28
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	8	0.28
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	8	0.28
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	8	0.28
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	8	0.28
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	8	0.28
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	8	0.28
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	8	0.28
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	8	0.28
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	8	0.28
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	8	0.28
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	8	0.28
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	8	0.28
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	8	0.28
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	8	0.28
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	8	0.28
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	10	0.28
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	10	0.28
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	10	0.28
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	10	0.28
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	10	0.28
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	10	0.28
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	10	0.28
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	10	0.28
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	10	0.28
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	2	0.28
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	2	0.28
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	2	0.28
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	2	0.28
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	2	0.28
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	2	0.28
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	2	0.28
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	2	0.28
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	2	0.28
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	7	0.28
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	7	0.28
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	7	0.28
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	7	0.28
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	7	0.28
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	7	0.28
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	7	0.28
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	7	0.28
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	7	0.28
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	4	0.28
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	4	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	4	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	4	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	4	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	4	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	4	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	4	0.28
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	6	0.28
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	6	0.28
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	6	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	6	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	6	0.28
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	6	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	6	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	6	0.28
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	6	0.28
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	6	0.28
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	6	0.28
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	6	0.28
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	6	0.28
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	6	0.28
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	6	0.28
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	6	0.28
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	6	0.28
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	6	0.28
(1,348)	1:146:A:GLU:H	1:191:A:LYS:H	2	0.28
(1,247)	1:35:A:ASN:H	1:38:A:TYR:H	9	0.28
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	2	0.27
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	2	0.27
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	2	0.27
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG11	6	0.27
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG12	6	0.27
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG13	6	0.27
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB1	6	0.27
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB2	6	0.27
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB3	6	0.27
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG21	5	0.27
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG22	5	0.27
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG23	5	0.27
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	10	0.27
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	10	0.27
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD11	9	0.27
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD12	9	0.27
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD13	9	0.27
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE1	3	0.27
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE2	3	0.27
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE3	3	0.27
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD11	9	0.27
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD12	9	0.27
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD13	9	0.27
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	1	0.27
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	1	0.27
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	1	0.27
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG21	6	0.27
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG22	6	0.27
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG23	6	0.27
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD21	8	0.27
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD22	8	0.27
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD23	8	0.27
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD11	2	0.27
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD12	2	0.27
(1,811)	1:83:A:ASN:H	1:198:A:LEU:HD13	2	0.27
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	10	0.27
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	10	0.27
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	10	0.27
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD11	8	0.27
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD12	8	0.27
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD13	8	0.27
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD11	8	0.27
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD12	8	0.27
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD13	8	0.27
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD11	8	0.27
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD12	8	0.27
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD13	8	0.27
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD11	8	0.27
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD12	8	0.27
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD13	8	0.27
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD21	1	0.27
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD22	1	0.27
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD23	1	0.27
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD21	1	0.27
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD22	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD23	1	0.27
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD21	1	0.27
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD22	1	0.27
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD23	1	0.27
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	8	0.27
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	8	0.27
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	8	0.27
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	8	0.27
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	8	0.27
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	8	0.27
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	8	0.27
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	8	0.27
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	8	0.27
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE1	2	0.27
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE2	2	0.27
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE3	2	0.27
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE1	2	0.27
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE2	2	0.27
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE3	2	0.27
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE1	2	0.27
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE2	2	0.27
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE3	2	0.27
(1,526)	1:98:A:MET:HE1	1:184:A:THR:HG21	1	0.27
(1,526)	1:98:A:MET:HE1	1:184:A:THR:HG22	1	0.27
(1,526)	1:98:A:MET:HE1	1:184:A:THR:HG23	1	0.27
(1,526)	1:98:A:MET:HE2	1:184:A:THR:HG21	1	0.27
(1,526)	1:98:A:MET:HE2	1:184:A:THR:HG22	1	0.27
(1,526)	1:98:A:MET:HE2	1:184:A:THR:HG23	1	0.27
(1,526)	1:98:A:MET:HE3	1:184:A:THR:HG21	1	0.27
(1,526)	1:98:A:MET:HE3	1:184:A:THR:HG22	1	0.27
(1,526)	1:98:A:MET:HE3	1:184:A:THR:HG23	1	0.27
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	2	0.27
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	2	0.27
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	2	0.27
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	2	0.27
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	2	0.27
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	2	0.27
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	2	0.27
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	2	0.27
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	2	0.27
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	5	0.27
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	5	0.27
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	5	0.27
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	5	0.27
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	5	0.27
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	5	0.27
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	5	0.27
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	5	0.27
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	3	0.27
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	3	0.27
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	3	0.27
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	3	0.27
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	3	0.27
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	3	0.27
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	3	0.27
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	3	0.27
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	3	0.27
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	5	0.27
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	5	0.27
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	5	0.27
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	5	0.27
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	5	0.27
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	5	0.27
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	5	0.27
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	5	0.27
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	5	0.27
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	4	0.27
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	4	0.27
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	4	0.27
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	4	0.27
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	4	0.27
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	4	0.27
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	4	0.27
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	4	0.27
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	4	0.27
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	7	0.27
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	7	0.27
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	7	0.27
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	7	0.27
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	7	0.27
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	7	0.27
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	7	0.27
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	7	0.27
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	5	0.27
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	5	0.27
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	5	0.27
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	5	0.27
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	5	0.27
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	5	0.27
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	5	0.27
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	5	0.27
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	5	0.27
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	2	0.27
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	2	0.27
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	2	0.27
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	2	0.27
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	2	0.27
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	2	0.27
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	2	0.27
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	2	0.27
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	2	0.27
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	6	0.27
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	6	0.27
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	6	0.27
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	6	0.27
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	6	0.27
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	6	0.27
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	6	0.27
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	6	0.27
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	6	0.27
(1,342)	1:103:A:LEU:H	1:107:A:LEU:H	4	0.27
(1,342)	1:103:A:LEU:H	1:107:A:LEU:H	8	0.27
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	1	0.27
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	7	0.27
(1,288)	1:196:A:GLU:H	1:199:A:GLU:H	4	0.27
(1,263)	1:70:A:LEU:H	1:73:A:GLY:H	4	0.27
(1,41)	1:76:A:LEU:H	1:77:A:HIS:H	9	0.27
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	3	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	3	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	3	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	7	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	7	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	7	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	9	0.26
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	9	0.26
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	1	0.26
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	1	0.26
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	1	0.26
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	9	0.26
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	9	0.26
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	9	0.26
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	4	0.26
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	4	0.26
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	4	0.26
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG21	3	0.26
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG22	3	0.26
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG23	3	0.26
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG21	3	0.26
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG22	3	0.26
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG23	3	0.26
(1,885)	1:127:A:ASP:H	1:126:A:ALA:HB1	8	0.26
(1,885)	1:127:A:ASP:H	1:126:A:ALA:HB2	8	0.26
(1,885)	1:127:A:ASP:H	1:126:A:ALA:HB3	8	0.26
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG21	1	0.26
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG22	1	0.26
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG23	1	0.26
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG21	9	0.26
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG22	9	0.26
(1,817)	1:86:A:ASP:H	1:88:A:THR:HG23	9	0.26
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	4	0.26
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	4	0.26
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	4	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	3	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	3	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	3	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	9	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	9	0.26
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	9	0.26
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD11	6	0.26
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD12	6	0.26
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD13	6	0.26
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	2	0.26
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	2	0.26
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	2	0.26
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	6	0.26
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	6	0.26
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	1	0.26
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	1	0.26
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	1	0.26
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	7	0.26
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	7	0.26
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	7	0.26
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	4	0.26
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	4	0.26
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	4	0.26
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	4	0.26
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	4	0.26
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	4	0.26
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	4	0.26
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	4	0.26
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	4	0.26
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	3	0.26
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	3	0.26
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	3	0.26
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	3	0.26
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	3	0.26
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	3	0.26
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	3	0.26
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	3	0.26
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	3	0.26
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD11	5	0.26
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD12	5	0.26
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD13	5	0.26
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD11	5	0.26
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD12	5	0.26
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD13	5	0.26
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD11	5	0.26
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD12	5	0.26
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD13	5	0.26
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	9	0.26
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	9	0.26
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	9	0.26
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	9	0.26
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	9	0.26
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	9	0.26
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	9	0.26
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	9	0.26
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	6	0.26
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	6	0.26
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	6	0.26
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	6	0.26
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	6	0.26
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	6	0.26
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	6	0.26
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	6	0.26
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	6	0.26
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	10	0.26
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	10	0.26
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	10	0.26
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	10	0.26
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	10	0.26
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	10	0.26
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	10	0.26
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	10	0.26
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	10	0.26
(1,498)	1:81:A:ILE:HD11	1:92:A:VAL:HG11	2	0.26
(1,498)	1:81:A:ILE:HD11	1:92:A:VAL:HG12	2	0.26
(1,498)	1:81:A:ILE:HD11	1:92:A:VAL:HG13	2	0.26
(1,498)	1:81:A:ILE:HD12	1:92:A:VAL:HG11	2	0.26
(1,498)	1:81:A:ILE:HD12	1:92:A:VAL:HG12	2	0.26
(1,498)	1:81:A:ILE:HD12	1:92:A:VAL:HG13	2	0.26
(1,498)	1:81:A:ILE:HD13	1:92:A:VAL:HG11	2	0.26
(1,498)	1:81:A:ILE:HD13	1:92:A:VAL:HG12	2	0.26
(1,498)	1:81:A:ILE:HD13	1:92:A:VAL:HG13	2	0.26
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	2	0.26
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	2	0.26
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	2	0.26
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	2	0.26
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	2	0.26
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	2	0.26
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	2	0.26
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	2	0.26
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	2	0.26
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	5	0.26
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	5	0.26
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	5	0.26
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	5	0.26
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	5	0.26
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	5	0.26
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	5	0.26
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	5	0.26
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	9	0.26
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	9	0.26
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	9	0.26
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	9	0.26
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	9	0.26
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	9	0.26
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	9	0.26
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	9	0.26
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	9	0.26
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	6	0.26
(1,340)	1:93:A:ASP:H	1:186:A:VAL:H	5	0.26
(1,247)	1:35:A:ASN:H	1:38:A:TYR:H	5	0.26
(1,40)	1:75:A:GLU:H	1:76:A:LEU:H	5	0.26
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG21	10	0.25
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG22	10	0.25
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG23	10	0.25
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	1	0.25
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	1	0.25
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	1	0.25
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD21	8	0.25
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD22	8	0.25
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD23	8	0.25
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG21	9	0.25
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG22	9	0.25
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG23	9	0.25
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD21	10	0.25
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD22	10	0.25
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD23	10	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	3	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	3	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	3	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	4	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	4	0.25
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	4	0.25
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	5	0.25
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	5	0.25
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	4	0.25
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	4	0.25
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	4	0.25
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	3	0.25
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	3	0.25
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	3	0.25
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	8	0.25
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	8	0.25
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	8	0.25
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG21	1	0.25
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG22	1	0.25
(1,899)	1:138:A:PHE:H	1:136:A:VAL:HG23	1	0.25
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB1	7	0.25
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB2	7	0.25
(1,870)	1:122:A:LEU:H	1:124:A:ALA:HB3	7	0.25
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB1	6	0.25
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB2	6	0.25
(1,865)	1:118:A:PHE:H	1:121:A:ALA:HB3	6	0.25
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	1	0.25
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	1	0.25
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	1	0.25
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD11	8	0.25
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD12	8	0.25
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD13	8	0.25
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD11	10	0.25
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD12	10	0.25
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD13	10	0.25
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	7	0.25
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	7	0.25
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	7	0.25
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD11	3	0.25
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD12	3	0.25
(1,609)	1:26:A:ILE:H	1:26:A:ILE:HD13	3	0.25
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD11	8	0.25
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD12	8	0.25
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD13	8	0.25
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD11	8	0.25
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD12	8	0.25
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD13	8	0.25
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD11	8	0.25
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD12	8	0.25
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD13	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	8	0.25
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	8	0.25
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	8	0.25
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	8	0.25
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	8	0.25
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	8	0.25
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	8	0.25
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	8	0.25
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	8	0.25
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	6	0.25
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	6	0.25
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	6	0.25
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	6	0.25
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	6	0.25
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	6	0.25
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	6	0.25
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	6	0.25
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	6	0.25
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	8	0.25
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	8	0.25
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	8	0.25
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	8	0.25
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	8	0.25
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	8	0.25
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	8	0.25
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	8	0.25
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	8	0.25
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	6	0.25
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	6	0.25
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	6	0.25
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	6	0.25
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	6	0.25
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	6	0.25
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	6	0.25
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	6	0.25
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	6	0.25
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD11	6	0.25
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD12	6	0.25
(1,480)	1:56:A:LEU:HD21	1:76:A:LEU:HD13	6	0.25
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD11	6	0.25
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD12	6	0.25
(1,480)	1:56:A:LEU:HD22	1:76:A:LEU:HD13	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD11	6	0.25
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD12	6	0.25
(1,480)	1:56:A:LEU:HD23	1:76:A:LEU:HD13	6	0.25
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	9	0.25
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	9	0.25
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	9	0.25
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	9	0.25
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	9	0.25
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	9	0.25
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	9	0.25
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	9	0.25
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	9	0.25
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	5	0.25
(1,57)	1:96:A:ILE:H	1:97:A:GLY:H	3	0.25
(2,98)	1:44:A:PHE:H	1:41:A:LYS:O	4	0.24
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	2	0.24
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	2	0.24
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	2	0.24
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	9	0.24
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	9	0.24
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	9	0.24
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	10	0.24
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	10	0.24
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	10	0.24
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	2	0.24
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	2	0.24
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	2	0.24
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG21	3	0.24
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG22	3	0.24
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG23	3	0.24
(1,1008)	1:187:A:ILE:H	1:150:A:VAL:HG21	2	0.24
(1,1008)	1:187:A:ILE:H	1:150:A:VAL:HG22	2	0.24
(1,1008)	1:187:A:ILE:H	1:150:A:VAL:HG23	2	0.24
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	8	0.24
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	8	0.24
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	8	0.24
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG21	8	0.24
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG22	8	0.24
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG23	8	0.24
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	10	0.24
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	10	0.24
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	1	0.24
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	1	0.24
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	1	0.24
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG21	6	0.24
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG22	6	0.24
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG23	6	0.24
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	6	0.24
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	6	0.24
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	6	0.24
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE1	2	0.24
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE2	2	0.24
(1,886)	1:127:A:ASP:H	1:130:A:MET:HE3	2	0.24
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB1	1	0.24
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB2	1	0.24
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB3	1	0.24
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	5	0.24
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	5	0.24
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	5	0.24
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG21	3	0.24
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG22	3	0.24
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG23	3	0.24
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD11	7	0.24
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD12	7	0.24
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD13	7	0.24
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	2	0.24
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	2	0.24
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	2	0.24
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	10	0.24
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	10	0.24
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	10	0.24
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	6	0.24
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	6	0.24
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	6	0.24
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	4	0.24
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	4	0.24
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	4	0.24
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG21	10	0.24
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG22	10	0.24
(1,685)	1:18:A:GLU:H	1:172:A:VAL:HG23	10	0.24
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG11	5	0.24
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG12	5	0.24
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG13	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD11	7	0.24
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD12	7	0.24
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD13	7	0.24
(1,628)	1:76:A:LEU:H	1:76:A:LEU:HD21	10	0.24
(1,628)	1:76:A:LEU:H	1:76:A:LEU:HD22	10	0.24
(1,628)	1:76:A:LEU:H	1:76:A:LEU:HD23	10	0.24
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD21	2	0.24
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD22	2	0.24
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD23	2	0.24
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD21	2	0.24
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD22	2	0.24
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD23	2	0.24
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD21	2	0.24
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD22	2	0.24
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD23	2	0.24
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	8	0.24
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	8	0.24
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	8	0.24
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	8	0.24
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	8	0.24
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	8	0.24
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	8	0.24
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	8	0.24
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	8	0.24
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG21	10	0.24
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG22	10	0.24
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG23	10	0.24
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG21	10	0.24
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG22	10	0.24
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG23	10	0.24
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG21	10	0.24
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG22	10	0.24
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG23	10	0.24
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	7	0.24
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	7	0.24
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	7	0.24
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	7	0.24
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	7	0.24
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	7	0.24
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	7	0.24
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	7	0.24
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG11	9	0.24
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG12	9	0.24
(1,577)	1:150:A:VAL:HG11	1:186:A:VAL:HG13	9	0.24
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG11	9	0.24
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG12	9	0.24
(1,577)	1:150:A:VAL:HG12	1:186:A:VAL:HG13	9	0.24
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG11	9	0.24
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG12	9	0.24
(1,577)	1:150:A:VAL:HG13	1:186:A:VAL:HG13	9	0.24
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	8	0.24
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	8	0.24
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	8	0.24
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	8	0.24
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	8	0.24
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	8	0.24
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	8	0.24
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	8	0.24
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	8	0.24
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	8	0.24
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	8	0.24
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	8	0.24
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	8	0.24
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	8	0.24
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	8	0.24
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	8	0.24
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	8	0.24
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	8	0.24
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	4	0.24
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	4	0.24
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	4	0.24
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	4	0.24
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	4	0.24
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	4	0.24
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	4	0.24
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	4	0.24
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	4	0.24
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	1	0.24
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	1	0.24
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	1	0.24
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	1	0.24
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	1	0.24
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	1	0.24
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	1	0.24
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	1	0.24
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG21	3	0.24
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG22	3	0.24
(1,474)	1:49:A:ILE:HD11	1:207:A:VAL:HG23	3	0.24
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG21	3	0.24
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG22	3	0.24
(1,474)	1:49:A:ILE:HD12	1:207:A:VAL:HG23	3	0.24
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG21	3	0.24
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG22	3	0.24
(1,474)	1:49:A:ILE:HD13	1:207:A:VAL:HG23	3	0.24
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	7	0.24
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	7	0.24
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	7	0.24
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	7	0.24
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	7	0.24
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	7	0.24
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	7	0.24
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	7	0.24
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	7	0.24
(1,374)	1:225:A:GLU:H	1:230:A:VAL:H	6	0.24
(1,360)	1:153:A:LYS:H	1:183:A:GLY:H	5	0.24
(1,340)	1:93:A:ASP:H	1:186:A:VAL:H	1	0.24
(1,262)	1:69:A:LYS:H	1:72:A:SER:H	4	0.24
(1,209)	1:137:A:GLY:H	1:139:A:TYR:H	3	0.24
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	6	0.23
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	6	0.23
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	6	0.23
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG11	10	0.23
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG12	10	0.23
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG13	10	0.23
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD11	5	0.23
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD12	5	0.23
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD13	5	0.23
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD11	6	0.23
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD12	6	0.23
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD13	6	0.23
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD21	9	0.23
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD22	9	0.23
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD23	9	0.23
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE1	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE2	10	0.23
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE3	10	0.23
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	10	0.23
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	10	0.23
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	10	0.23
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	4	0.23
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	4	0.23
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	4	0.23
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG21	7	0.23
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG22	7	0.23
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG23	7	0.23
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG21	7	0.23
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG22	7	0.23
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG23	7	0.23
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG21	2	0.23
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG22	2	0.23
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG23	2	0.23
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	4	0.23
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	4	0.23
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	4	0.23
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	3	0.23
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	3	0.23
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	3	0.23
(1,822)	1:87:A:ARG:H	1:198:A:LEU:HD21	8	0.23
(1,822)	1:87:A:ARG:H	1:198:A:LEU:HD22	8	0.23
(1,822)	1:87:A:ARG:H	1:198:A:LEU:HD23	8	0.23
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	6	0.23
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	6	0.23
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	6	0.23
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD11	9	0.23
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD12	9	0.23
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD13	9	0.23
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD21	4	0.23
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD22	4	0.23
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD23	4	0.23
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD21	2	0.23
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD22	2	0.23
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD23	2	0.23
(1,736)	1:49:A:ILE:H	1:80:A:LEU:HD21	8	0.23
(1,736)	1:49:A:ILE:H	1:80:A:LEU:HD22	8	0.23
(1,736)	1:49:A:ILE:H	1:80:A:LEU:HD23	8	0.23
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG11	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG12	3	0.23
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG13	3	0.23
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	7	0.23
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	7	0.23
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	7	0.23
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	3	0.23
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	3	0.23
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	3	0.23
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	3	0.23
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	3	0.23
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	3	0.23
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	2	0.23
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	2	0.23
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	2	0.23
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	1	0.23
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	1	0.23
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	1	0.23
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	1	0.23
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	1	0.23
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	1	0.23
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	1	0.23
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	1	0.23
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	1	0.23
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	5	0.23
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	5	0.23
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	5	0.23
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	5	0.23
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	5	0.23
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	5	0.23
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	5	0.23
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	5	0.23
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	5	0.23
(1,514)	1:91:A:ILE:HD11	1:188:A:LEU:HD21	3	0.23
(1,514)	1:91:A:ILE:HD11	1:188:A:LEU:HD22	3	0.23
(1,514)	1:91:A:ILE:HD11	1:188:A:LEU:HD23	3	0.23
(1,514)	1:91:A:ILE:HD12	1:188:A:LEU:HD21	3	0.23
(1,514)	1:91:A:ILE:HD12	1:188:A:LEU:HD22	3	0.23
(1,514)	1:91:A:ILE:HD12	1:188:A:LEU:HD23	3	0.23
(1,514)	1:91:A:ILE:HD13	1:188:A:LEU:HD21	3	0.23
(1,514)	1:91:A:ILE:HD13	1:188:A:LEU:HD22	3	0.23
(1,514)	1:91:A:ILE:HD13	1:188:A:LEU:HD23	3	0.23
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	10	0.23
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	10	0.23
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	10	0.23
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	10	0.23
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	10	0.23
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	10	0.23
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	10	0.23
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	10	0.23
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	6	0.23
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	6	0.23
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	6	0.23
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	6	0.23
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	6	0.23
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	6	0.23
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	6	0.23
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	6	0.23
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	6	0.23
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG21	3	0.23
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG22	3	0.23
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG23	3	0.23
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG21	3	0.23
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG22	3	0.23
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG23	3	0.23
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG21	3	0.23
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG22	3	0.23
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG23	3	0.23
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	7	0.23
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	7	0.23
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	7	0.23
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	7	0.23
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	7	0.23
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	7	0.23
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	7	0.23
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	7	0.23
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	7	0.23
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG11	8	0.23
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG12	8	0.23
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG13	8	0.23
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG11	8	0.23
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG12	8	0.23
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG13	8	0.23
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG11	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG12	8	0.23
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG13	8	0.23
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	10	0.23
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	10	0.23
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	10	0.23
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	10	0.23
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	10	0.23
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	10	0.23
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	10	0.23
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	10	0.23
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	10	0.23
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	8	0.23
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	8	0.23
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	8	0.23
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	8	0.23
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	8	0.23
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	8	0.23
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	8	0.23
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	8	0.23
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	8	0.23
(1,362)	1:159:A:GLN:H	1:175:A:ASP:H	3	0.23
(1,184)	1:72:A:SER:H	1:74:A:LYS:H	3	0.23
(1,101)	1:168:A:GLY:H	1:169:A:SER:H	6	0.23
(1,84)	1:144:A:VAL:H	1:145:A:ALA:H	2	0.23
(1,79)	1:137:A:GLY:H	1:138:A:PHE:H	3	0.23
(1,79)	1:137:A:GLY:H	1:138:A:PHE:H	7	0.23
(1,11)	1:41:A:LYS:H	1:42:A:GLU:H	4	0.23
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD11	8	0.22
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD12	8	0.22
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD13	8	0.22
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD11	4	0.22
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD12	4	0.22
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD13	4	0.22
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD21	8	0.22
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD22	8	0.22
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD23	8	0.22
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD21	5	0.22
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD22	5	0.22
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD23	5	0.22
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	10	0.22
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	10	0.22
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	4	0.22
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	4	0.22
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	4	0.22
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	5	0.22
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	5	0.22
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	5	0.22
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG21	3	0.22
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG22	3	0.22
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG23	3	0.22
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	6	0.22
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	6	0.22
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	6	0.22
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	4	0.22
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	4	0.22
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	4	0.22
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	10	0.22
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	10	0.22
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	10	0.22
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG21	3	0.22
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG22	3	0.22
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG23	3	0.22
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG21	7	0.22
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG22	7	0.22
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG23	7	0.22
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD21	3	0.22
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD22	3	0.22
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD23	3	0.22
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	7	0.22
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	7	0.22
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	7	0.22
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB1	2	0.22
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB2	2	0.22
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB3	2	0.22
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	5	0.22
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	5	0.22
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	5	0.22
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG11	7	0.22
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG12	7	0.22
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG13	7	0.22
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	10	0.22
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	10	0.22
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	10	0.22
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	10	0.22
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	10	0.22
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	10	0.22
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	10	0.22
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	10	0.22
(1,568)	1:144:A:VAL:HG21	1:188:A:LEU:HD21	3	0.22
(1,568)	1:144:A:VAL:HG21	1:188:A:LEU:HD22	3	0.22
(1,568)	1:144:A:VAL:HG21	1:188:A:LEU:HD23	3	0.22
(1,568)	1:144:A:VAL:HG22	1:188:A:LEU:HD21	3	0.22
(1,568)	1:144:A:VAL:HG22	1:188:A:LEU:HD22	3	0.22
(1,568)	1:144:A:VAL:HG22	1:188:A:LEU:HD23	3	0.22
(1,568)	1:144:A:VAL:HG23	1:188:A:LEU:HD21	3	0.22
(1,568)	1:144:A:VAL:HG23	1:188:A:LEU:HD22	3	0.22
(1,568)	1:144:A:VAL:HG23	1:188:A:LEU:HD23	3	0.22
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	6	0.22
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	6	0.22
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	6	0.22
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	6	0.22
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	6	0.22
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	6	0.22
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	6	0.22
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	6	0.22
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	6	0.22
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	9	0.22
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	9	0.22
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	9	0.22
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	9	0.22
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	9	0.22
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	9	0.22
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	9	0.22
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	9	0.22
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	9	0.22
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	7	0.22
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	7	0.22
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	7	0.22
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	7	0.22
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	7	0.22
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	7	0.22
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	7	0.22
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	7	0.22
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD11	1	0.22
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD12	1	0.22
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD13	1	0.22
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD11	1	0.22
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD12	1	0.22
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD13	1	0.22
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD11	1	0.22
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD12	1	0.22
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD13	1	0.22
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD11	3	0.22
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD12	3	0.22
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD13	3	0.22
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD11	3	0.22
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD12	3	0.22
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD13	3	0.22
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD11	3	0.22
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD12	3	0.22
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD13	3	0.22
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG21	5	0.22
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG22	5	0.22
(1,497)	1:81:A:ILE:HD11	1:90:A:THR:HG23	5	0.22
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG21	5	0.22
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG22	5	0.22
(1,497)	1:81:A:ILE:HD12	1:90:A:THR:HG23	5	0.22
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG21	5	0.22
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG22	5	0.22
(1,497)	1:81:A:ILE:HD13	1:90:A:THR:HG23	5	0.22
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	7	0.22
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	7	0.22
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	7	0.22
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	7	0.22
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	7	0.22
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	7	0.22
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	7	0.22
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	7	0.22
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	7	0.22
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG11	1	0.22
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG12	1	0.22
(1,473)	1:49:A:ILE:HD11	1:207:A:VAL:HG13	1	0.22
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG11	1	0.22
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG12	1	0.22
(1,473)	1:49:A:ILE:HD12	1:207:A:VAL:HG13	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG11	1	0.22
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG12	1	0.22
(1,473)	1:49:A:ILE:HD13	1:207:A:VAL:HG13	1	0.22
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	4	0.22
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	4	0.22
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	4	0.22
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	4	0.22
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	4	0.22
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	4	0.22
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	4	0.22
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	4	0.22
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	4	0.22
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	8	0.22
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	8	0.22
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	8	0.22
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	8	0.22
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	8	0.22
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	8	0.22
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	8	0.22
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	8	0.22
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	8	0.22
(1,341)	1:95:A:GLY:H	1:184:A:THR:H	10	0.22
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	10	0.22
(1,288)	1:196:A:GLU:H	1:199:A:GLU:H	6	0.22
(1,267)	1:99:A:THR:H	1:102:A:ASP:H	6	0.22
(1,139)	1:212:A:GLN:H	1:213:A:PHE:H	5	0.22
(1,79)	1:137:A:GLY:H	1:138:A:PHE:H	4	0.22
(1,79)	1:137:A:GLY:H	1:138:A:PHE:H	10	0.22
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD11	2	0.21
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD12	2	0.21
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD13	2	0.21
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	7	0.21
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	7	0.21
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	7	0.21
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	6	0.21
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	6	0.21
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	6	0.21
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG21	8	0.21
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG22	8	0.21
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG23	8	0.21
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD21	5	0.21
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD22	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD23	5	0.21
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	8	0.21
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	8	0.21
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	8	0.21
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG21	3	0.21
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG22	3	0.21
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG23	3	0.21
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD11	4	0.21
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD12	4	0.21
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD13	4	0.21
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG21	2	0.21
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG22	2	0.21
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG23	2	0.21
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	3	0.21
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	3	0.21
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	3	0.21
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG21	7	0.21
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG22	7	0.21
(1,946)	1:151:A:ILE:H	1:186:A:VAL:HG23	7	0.21
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	9	0.21
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	9	0.21
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	9	0.21
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	2	0.21
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	2	0.21
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	2	0.21
(1,828)	1:89:A:LEU:H	1:198:A:LEU:HD21	8	0.21
(1,828)	1:89:A:LEU:H	1:198:A:LEU:HD22	8	0.21
(1,828)	1:89:A:LEU:H	1:198:A:LEU:HD23	8	0.21
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD11	1	0.21
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD12	1	0.21
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD13	1	0.21
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	10	0.21
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	10	0.21
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	10	0.21
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	5	0.21
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	5	0.21
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	5	0.21
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD11	10	0.21
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD12	10	0.21
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD13	10	0.21
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG11	7	0.21
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG12	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG13	7	0.21
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD11	4	0.21
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD12	4	0.21
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD13	4	0.21
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG21	10	0.21
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG22	10	0.21
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG23	10	0.21
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD21	7	0.21
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD22	7	0.21
(1,590)	1:188:A:LEU:HD11	1:190:A:LEU:HD23	7	0.21
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD21	7	0.21
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD22	7	0.21
(1,590)	1:188:A:LEU:HD12	1:190:A:LEU:HD23	7	0.21
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD21	7	0.21
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD22	7	0.21
(1,590)	1:188:A:LEU:HD13	1:190:A:LEU:HD23	7	0.21
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD11	4	0.21
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD12	4	0.21
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD13	4	0.21
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD11	4	0.21
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD12	4	0.21
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD13	4	0.21
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD11	4	0.21
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD12	4	0.21
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD13	4	0.21
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	8	0.21
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	8	0.21
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	8	0.21
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	8	0.21
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	8	0.21
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	8	0.21
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	8	0.21
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	8	0.21
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	8	0.21
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE1	7	0.21
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE2	7	0.21
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE3	7	0.21
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE1	7	0.21
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE2	7	0.21
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE3	7	0.21
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE1	7	0.21
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE3	7	0.21
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	3	0.21
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	3	0.21
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	3	0.21
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	3	0.21
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	3	0.21
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	3	0.21
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	3	0.21
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	3	0.21
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	3	0.21
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	10	0.21
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	10	0.21
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	10	0.21
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	10	0.21
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	10	0.21
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	10	0.21
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	10	0.21
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	10	0.21
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	10	0.21
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	1	0.21
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	1	0.21
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	1	0.21
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	1	0.21
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	1	0.21
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	1	0.21
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	1	0.21
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	1	0.21
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	1	0.21
(1,452)	1:45:A:LEU:HD21	1:48:A:LEU:HD21	9	0.21
(1,452)	1:45:A:LEU:HD21	1:48:A:LEU:HD22	9	0.21
(1,452)	1:45:A:LEU:HD21	1:48:A:LEU:HD23	9	0.21
(1,452)	1:45:A:LEU:HD22	1:48:A:LEU:HD21	9	0.21
(1,452)	1:45:A:LEU:HD22	1:48:A:LEU:HD22	9	0.21
(1,452)	1:45:A:LEU:HD22	1:48:A:LEU:HD23	9	0.21
(1,452)	1:45:A:LEU:HD23	1:48:A:LEU:HD21	9	0.21
(1,452)	1:45:A:LEU:HD23	1:48:A:LEU:HD22	9	0.21
(1,452)	1:45:A:LEU:HD23	1:48:A:LEU:HD23	9	0.21
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	7	0.21
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	7	0.21
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	7	0.21
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	7	0.21
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	7	0.21
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	7	0.21
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	7	0.21
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	7	0.21
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	8	0.21
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	8	0.21
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	8	0.21
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	8	0.21
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	8	0.21
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	8	0.21
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	8	0.21
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	8	0.21
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	8	0.21
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG21	3	0.21
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG22	3	0.21
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG23	3	0.21
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG21	3	0.21
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG22	3	0.21
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG23	3	0.21
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG21	3	0.21
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG22	3	0.21
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG23	3	0.21
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD11	2	0.21
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD12	2	0.21
(1,415)	1:29:A:LEU:HD11	1:122:A:LEU:HD13	2	0.21
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD11	2	0.21
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD12	2	0.21
(1,415)	1:29:A:LEU:HD12	1:122:A:LEU:HD13	2	0.21
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD11	2	0.21
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD12	2	0.21
(1,415)	1:29:A:LEU:HD13	1:122:A:LEU:HD13	2	0.21
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	3	0.21
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	3	0.21
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	3	0.21
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	3	0.21
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	3	0.21
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	3	0.21
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	3	0.21
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	3	0.21
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	3	0.21
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	1	0.21
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:159:A:GLN:H	1:175:A:ASP:H	4	0.21
(1,343)	1:114:A:GLY:H	1:118:A:PHE:H	1	0.21
(1,242)	1:223:A:GLU:H	1:225:A:GLU:H	1	0.21
(1,242)	1:223:A:GLU:H	1:225:A:GLU:H	3	0.21
(1,217)	1:180:A:MET:H	1:182:A:ARG:H	9	0.21
(1,208)	1:136:A:VAL:H	1:138:A:PHE:H	10	0.21
(1,40)	1:75:A:GLU:H	1:76:A:LEU:H	9	0.21
(2,150)	1:211:A:SER:H	1:207:A:VAL:O	8	0.2
(2,96)	1:35:A:ASN:H	1:31:A:SER:O	8	0.2
(2,80)	1:190:A:LEU:H	1:87:A:ARG:O	9	0.2
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	2	0.2
(2,2)	1:18:A:GLU:H	1:172:A:VAL:O	9	0.2
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG11	6	0.2
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG12	6	0.2
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG13	6	0.2
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD11	1	0.2
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD12	1	0.2
(1,1109)	1:222:A:VAL:H	1:220:A:LEU:HD13	1	0.2
(1,1100)	1:221:A:PHE:H	1:80:A:LEU:HD11	1	0.2
(1,1100)	1:221:A:PHE:H	1:80:A:LEU:HD12	1	0.2
(1,1100)	1:221:A:PHE:H	1:80:A:LEU:HD13	1	0.2
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD11	5	0.2
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD12	5	0.2
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD13	5	0.2
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG21	3	0.2
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG22	3	0.2
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG23	3	0.2
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	6	0.2
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	6	0.2
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	6	0.2
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	6	0.2
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	6	0.2
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	6	0.2
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	5	0.2
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	5	0.2
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	5	0.2
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG11	3	0.2
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG12	3	0.2
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG13	3	0.2
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG21	4	0.2
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG22	4	0.2
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG23	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE1	4	0.2
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE2	4	0.2
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE3	4	0.2
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	9	0.2
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	9	0.2
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	9	0.2
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG21	3	0.2
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG22	3	0.2
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG23	3	0.2
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	3	0.2
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	3	0.2
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	3	0.2
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG21	6	0.2
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG22	6	0.2
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG23	6	0.2
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	8	0.2
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	8	0.2
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	8	0.2
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	4	0.2
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	4	0.2
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	4	0.2
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	5	0.2
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	5	0.2
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	5	0.2
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG21	3	0.2
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG22	3	0.2
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG23	3	0.2
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD11	7	0.2
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD12	7	0.2
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD13	7	0.2
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	9	0.2
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	9	0.2
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	9	0.2
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG21	10	0.2
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG22	10	0.2
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG23	10	0.2
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	9	0.2
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	9	0.2
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	9	0.2
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	7	0.2
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	7	0.2
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG21	2	0.2
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG22	2	0.2
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG23	2	0.2
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	5	0.2
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	5	0.2
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	5	0.2
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD11	6	0.2
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD12	6	0.2
(1,792)	1:79:A:ASN:H	1:81:A:ILE:HD13	6	0.2
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD21	7	0.2
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD22	7	0.2
(1,778)	1:74:A:LYS:H	1:70:A:LEU:HD23	7	0.2
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD11	4	0.2
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD12	4	0.2
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD13	4	0.2
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD21	8	0.2
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD22	8	0.2
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD23	8	0.2
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	3	0.2
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	3	0.2
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	3	0.2
(1,725)	1:44:A:PHE:H	1:144:A:VAL:HG11	3	0.2
(1,725)	1:44:A:PHE:H	1:144:A:VAL:HG12	3	0.2
(1,725)	1:44:A:PHE:H	1:144:A:VAL:HG13	3	0.2
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	3	0.2
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	3	0.2
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	3	0.2
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG21	9	0.2
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG22	9	0.2
(1,660)	1:172:A:VAL:H	1:172:A:VAL:HG23	9	0.2
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD11	1	0.2
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD12	1	0.2
(1,644)	1:122:A:LEU:H	1:122:A:LEU:HD13	1	0.2
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	3	0.2
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	3	0.2
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	3	0.2
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	3	0.2
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	3	0.2
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	3	0.2
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	3	0.2
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	3	0.2
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE1	5	0.2
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE2	5	0.2
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE3	5	0.2
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE1	5	0.2
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE2	5	0.2
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE3	5	0.2
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE1	5	0.2
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE2	5	0.2
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE3	5	0.2
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	4	0.2
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	4	0.2
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	4	0.2
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	4	0.2
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	4	0.2
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	4	0.2
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	4	0.2
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	4	0.2
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	4	0.2
(1,535)	1:103:A:LEU:HD21	1:150:A:VAL:HG11	2	0.2
(1,535)	1:103:A:LEU:HD21	1:150:A:VAL:HG12	2	0.2
(1,535)	1:103:A:LEU:HD21	1:150:A:VAL:HG13	2	0.2
(1,535)	1:103:A:LEU:HD22	1:150:A:VAL:HG11	2	0.2
(1,535)	1:103:A:LEU:HD22	1:150:A:VAL:HG12	2	0.2
(1,535)	1:103:A:LEU:HD22	1:150:A:VAL:HG13	2	0.2
(1,535)	1:103:A:LEU:HD23	1:150:A:VAL:HG11	2	0.2
(1,535)	1:103:A:LEU:HD23	1:150:A:VAL:HG12	2	0.2
(1,535)	1:103:A:LEU:HD23	1:150:A:VAL:HG13	2	0.2
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	9	0.2
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	9	0.2
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	9	0.2
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	9	0.2
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	9	0.2
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	9	0.2
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	9	0.2
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	9	0.2
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	9	0.2
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG11	3	0.2
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG12	3	0.2
(1,511)	1:91:A:ILE:HD11	1:186:A:VAL:HG13	3	0.2
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG11	3	0.2
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG12	3	0.2
(1,511)	1:91:A:ILE:HD12	1:186:A:VAL:HG13	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG11	3	0.2
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG12	3	0.2
(1,511)	1:91:A:ILE:HD13	1:186:A:VAL:HG13	3	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	5	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	5	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	5	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	5	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	5	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	5	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	5	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	5	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	5	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	9	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	9	0.2
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	9	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	9	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	9	0.2
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	9	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	9	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	9	0.2
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	9	0.2
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	4	0.2
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	4	0.2
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	4	0.2
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	4	0.2
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	4	0.2
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	4	0.2
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	4	0.2
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	4	0.2
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	4	0.2
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	7	0.2
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	7	0.2
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	7	0.2
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	7	0.2
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	7	0.2
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	7	0.2
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	7	0.2
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	7	0.2
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	7	0.2
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD11	4	0.2
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD12	4	0.2
(1,478)	1:56:A:LEU:HD11	1:78:A:ILE:HD13	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD11	4	0.2
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD12	4	0.2
(1,478)	1:56:A:LEU:HD12	1:78:A:ILE:HD13	4	0.2
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD11	4	0.2
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD12	4	0.2
(1,478)	1:56:A:LEU:HD13	1:78:A:ILE:HD13	4	0.2
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB1	7	0.2
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB2	7	0.2
(1,439)	1:34:A:ILE:HD11	1:166:A:ALA:HB3	7	0.2
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB1	7	0.2
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB2	7	0.2
(1,439)	1:34:A:ILE:HD12	1:166:A:ALA:HB3	7	0.2
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB1	7	0.2
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB2	7	0.2
(1,439)	1:34:A:ILE:HD13	1:166:A:ALA:HB3	7	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	6	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	6	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	6	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	6	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	6	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	6	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	6	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	6	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	6	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	9	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	9	0.2
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	9	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	9	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	9	0.2
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	9	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	9	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	9	0.2
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	9	0.2
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	5	0.2
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	5	0.2
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	5	0.2
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	5	0.2
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	5	0.2
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	5	0.2
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	5	0.2
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	5	0.2
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG21	3	0.2
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG22	3	0.2
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG23	3	0.2
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG21	3	0.2
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG22	3	0.2
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG23	3	0.2
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG21	3	0.2
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG22	3	0.2
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG23	3	0.2
(1,298)	1:209:A:LYS:H	1:212:A:GLN:H	6	0.2
(2,148)	1:210:A:HIS:H	1:206:A:ILE:O	5	0.19
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	4	0.19
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG21	7	0.19
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG22	7	0.19
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG23	7	0.19
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD11	4	0.19
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD12	4	0.19
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD13	4	0.19
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG21	9	0.19
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG22	9	0.19
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG23	9	0.19
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	7	0.19
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	7	0.19
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	7	0.19
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	9	0.19
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	9	0.19
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	9	0.19
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD11	5	0.19
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD12	5	0.19
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD13	5	0.19
(1,1057)	1:200:A:GLU:H	1:220:A:LEU:HD21	2	0.19
(1,1057)	1:200:A:GLU:H	1:220:A:LEU:HD22	2	0.19
(1,1057)	1:200:A:GLU:H	1:220:A:LEU:HD23	2	0.19
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG21	3	0.19
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG22	3	0.19
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG23	3	0.19
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD21	8	0.19
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD22	8	0.19
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD23	8	0.19
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	5	0.19
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	5	0.19
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG21	8	0.19
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG22	8	0.19
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG23	8	0.19
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG21	1	0.19
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG22	1	0.19
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG23	1	0.19
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD11	9	0.19
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD12	9	0.19
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD13	9	0.19
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG21	5	0.19
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG22	5	0.19
(1,943)	1:151:A:ILE:H	1:150:A:VAL:HG23	5	0.19
(1,927)	1:146:A:GLU:H	1:145:A:ALA:HB1	3	0.19
(1,927)	1:146:A:GLU:H	1:145:A:ALA:HB2	3	0.19
(1,927)	1:146:A:GLU:H	1:145:A:ALA:HB3	3	0.19
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD11	3	0.19
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD12	3	0.19
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD13	3	0.19
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB1	9	0.19
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB2	9	0.19
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB3	9	0.19
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	4	0.19
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	4	0.19
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	4	0.19
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	10	0.19
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	10	0.19
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	10	0.19
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG21	6	0.19
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG22	6	0.19
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG23	6	0.19
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD11	2	0.19
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD12	2	0.19
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD13	2	0.19
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD21	3	0.19
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD22	3	0.19
(1,781)	1:75:A:GLU:H	1:70:A:LEU:HD23	3	0.19
(1,764)	1:62:A:GLU:H	1:96:A:ILE:HD11	6	0.19
(1,764)	1:62:A:GLU:H	1:96:A:ILE:HD12	6	0.19
(1,764)	1:62:A:GLU:H	1:96:A:ILE:HD13	6	0.19
(1,760)	1:61:A:TYR:H	1:76:A:LEU:HD11	4	0.19
(1,760)	1:61:A:TYR:H	1:76:A:LEU:HD12	4	0.19
(1,760)	1:61:A:TYR:H	1:76:A:LEU:HD13	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD21	3	0.19
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD22	3	0.19
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD23	3	0.19
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	2	0.19
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	2	0.19
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	2	0.19
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	1	0.19
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	1	0.19
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	1	0.19
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	4	0.19
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	4	0.19
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	4	0.19
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	10	0.19
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	10	0.19
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	10	0.19
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG21	10	0.19
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG22	10	0.19
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG23	10	0.19
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG21	8	0.19
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG22	8	0.19
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG23	8	0.19
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	5	0.19
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	5	0.19
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	5	0.19
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	9	0.19
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	9	0.19
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	9	0.19
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD11	5	0.19
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD12	5	0.19
(1,670)	1:203:A:ILE:H	1:203:A:ILE:HD13	5	0.19
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	5	0.19
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	5	0.19
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	5	0.19
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	5	0.19
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	5	0.19
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	5	0.19
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	5	0.19
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	5	0.19
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	5	0.19
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD11	6	0.19
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD12	6	0.19
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD13	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD11	6	0.19
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD12	6	0.19
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD13	6	0.19
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD11	6	0.19
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD12	6	0.19
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD13	6	0.19
(1,562)	1:141:A:ALA:HB1	1:186:A:VAL:HG11	4	0.19
(1,562)	1:141:A:ALA:HB1	1:186:A:VAL:HG12	4	0.19
(1,562)	1:141:A:ALA:HB1	1:186:A:VAL:HG13	4	0.19
(1,562)	1:141:A:ALA:HB2	1:186:A:VAL:HG11	4	0.19
(1,562)	1:141:A:ALA:HB2	1:186:A:VAL:HG12	4	0.19
(1,562)	1:141:A:ALA:HB2	1:186:A:VAL:HG13	4	0.19
(1,562)	1:141:A:ALA:HB3	1:186:A:VAL:HG11	4	0.19
(1,562)	1:141:A:ALA:HB3	1:186:A:VAL:HG12	4	0.19
(1,562)	1:141:A:ALA:HB3	1:186:A:VAL:HG13	4	0.19
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	7	0.19
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	7	0.19
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	7	0.19
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	7	0.19
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	7	0.19
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	7	0.19
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	7	0.19
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	7	0.19
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	7	0.19
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	6	0.19
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	6	0.19
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	6	0.19
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	6	0.19
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	6	0.19
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	6	0.19
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	6	0.19
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	6	0.19
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	6	0.19
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	1	0.19
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	1	0.19
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	1	0.19
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	1	0.19
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	1	0.19
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	1	0.19
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	1	0.19
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	1	0.19
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD11	8	0.19
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD12	8	0.19
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD13	8	0.19
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD11	8	0.19
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD12	8	0.19
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD13	8	0.19
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD11	8	0.19
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD12	8	0.19
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD13	8	0.19
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	7	0.19
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	7	0.19
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	7	0.19
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	7	0.19
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	7	0.19
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	7	0.19
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	7	0.19
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	7	0.19
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	7	0.19
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	5	0.19
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	5	0.19
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	5	0.19
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	5	0.19
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	5	0.19
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	5	0.19
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	5	0.19
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	5	0.19
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	5	0.19
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	8	0.19
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	8	0.19
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	8	0.19
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	8	0.19
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	8	0.19
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	8	0.19
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	8	0.19
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	8	0.19
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	8	0.19
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	4	0.19
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	4	0.19
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	4	0.19
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	4	0.19
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	4	0.19
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	4	0.19
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	4	0.19
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	4	0.19
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	4	0.19
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	4	0.19
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	4	0.19
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	4	0.19
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	4	0.19
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	4	0.19
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	4	0.19
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	4	0.19
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	4	0.19
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG21	9	0.19
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG22	9	0.19
(1,405)	1:19:A:THR:HG21	1:171:A:THR:HG23	9	0.19
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG21	9	0.19
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG22	9	0.19
(1,405)	1:19:A:THR:HG22	1:171:A:THR:HG23	9	0.19
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG21	9	0.19
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG22	9	0.19
(1,405)	1:19:A:THR:HG23	1:171:A:THR:HG23	9	0.19
(1,353)	1:149:A:THR:H	1:187:A:ILE:H	10	0.19
(1,317)	1:77:A:HIS:H	1:94:A:THR:H	5	0.19
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	4	0.19
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	1	0.19
(1,287)	1:194:A:GLN:H	1:197:A:TYR:H	1	0.19
(1,282)	1:138:A:PHE:H	1:141:A:ALA:H	2	0.19
(1,247)	1:35:A:ASN:H	1:38:A:TYR:H	3	0.19
(1,122)	1:195:A:THR:H	1:196:A:GLU:H	8	0.19
(2,28)	1:83:A:ASN:H	1:88:A:THR:O	6	0.18
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG11	7	0.18
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG12	7	0.18
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG13	7	0.18
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	3	0.18
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	3	0.18
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	3	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG21	1	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG22	1	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG23	1	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG21	3	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG22	3	0.18
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG23	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG11	7	0.18
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG12	7	0.18
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG13	7	0.18
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD11	7	0.18
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD12	7	0.18
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD13	7	0.18
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD11	10	0.18
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD12	10	0.18
(1,1066)	1:204:A:LYS:H	1:45:A:LEU:HD13	10	0.18
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD11	3	0.18
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD12	3	0.18
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD13	3	0.18
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD21	10	0.18
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD22	10	0.18
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD23	10	0.18
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD21	6	0.18
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD22	6	0.18
(1,1026)	1:189:A:HIS:H	1:188:A:LEU:HD23	6	0.18
(1,1024)	1:189:A:HIS:H	1:148:A:VAL:HG11	3	0.18
(1,1024)	1:189:A:HIS:H	1:148:A:VAL:HG12	3	0.18
(1,1024)	1:189:A:HIS:H	1:148:A:VAL:HG13	3	0.18
(1,1022)	1:189:A:HIS:H	1:88:A:THR:HG21	10	0.18
(1,1022)	1:189:A:HIS:H	1:88:A:THR:HG22	10	0.18
(1,1022)	1:189:A:HIS:H	1:88:A:THR:HG23	10	0.18
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD21	3	0.18
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD22	3	0.18
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD23	3	0.18
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	1	0.18
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	1	0.18
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	1	0.18
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	9	0.18
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	9	0.18
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	9	0.18
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD11	4	0.18
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD12	4	0.18
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD13	4	0.18
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG11	3	0.18
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG12	3	0.18
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG13	3	0.18
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD11	4	0.18
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD12	4	0.18
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD13	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD11	7	0.18
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD12	7	0.18
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD13	7	0.18
(1,863)	1:118:A:PHE:H	1:115:A:THR:HG21	7	0.18
(1,863)	1:118:A:PHE:H	1:115:A:THR:HG22	7	0.18
(1,863)	1:118:A:PHE:H	1:115:A:THR:HG23	7	0.18
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD21	5	0.18
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD22	5	0.18
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD23	5	0.18
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD11	3	0.18
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD12	3	0.18
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD13	3	0.18
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	10	0.18
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	10	0.18
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	10	0.18
(1,815)	1:85:A:GLN:H	1:198:A:LEU:HD11	7	0.18
(1,815)	1:85:A:GLN:H	1:198:A:LEU:HD12	7	0.18
(1,815)	1:85:A:GLN:H	1:198:A:LEU:HD13	7	0.18
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD11	9	0.18
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD12	9	0.18
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD13	9	0.18
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG21	3	0.18
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG22	3	0.18
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG23	3	0.18
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD11	10	0.18
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD12	10	0.18
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD13	10	0.18
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD11	8	0.18
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD12	8	0.18
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD13	8	0.18
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD21	7	0.18
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD22	7	0.18
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD23	7	0.18
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD11	5	0.18
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD12	5	0.18
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD13	5	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	1	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	1	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	1	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	10	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	10	0.18
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD11	2	0.18
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD12	2	0.18
(1,718)	1:42:A:GLU:H	1:143:A:LEU:HD13	2	0.18
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	7	0.18
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	7	0.18
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	7	0.18
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	9	0.18
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	9	0.18
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	9	0.18
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	7	0.18
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	7	0.18
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	7	0.18
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	9	0.18
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	9	0.18
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	9	0.18
(1,695)	1:27:A:ALA:H	1:26:A:ILE:HD11	2	0.18
(1,695)	1:27:A:ALA:H	1:26:A:ILE:HD12	2	0.18
(1,695)	1:27:A:ALA:H	1:26:A:ILE:HD13	2	0.18
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	6	0.18
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	6	0.18
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	6	0.18
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG11	4	0.18
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG12	4	0.18
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG13	4	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG21	4	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG22	4	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG23	4	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG21	9	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG22	9	0.18
(1,687)	1:20:A:PHE:H	1:171:A:THR:HG23	9	0.18
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	6	0.18
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	6	0.18
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	6	0.18
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	10	0.18
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	10	0.18
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	10	0.18
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	8	0.18
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	8	0.18
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	8	0.18
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	8	0.18
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	8	0.18
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	8	0.18
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	8	0.18
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	8	0.18
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD21	3	0.18
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD22	3	0.18
(1,566)	1:144:A:VAL:HG11	1:190:A:LEU:HD23	3	0.18
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD21	3	0.18
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD22	3	0.18
(1,566)	1:144:A:VAL:HG12	1:190:A:LEU:HD23	3	0.18
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD21	3	0.18
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD22	3	0.18
(1,566)	1:144:A:VAL:HG13	1:190:A:LEU:HD23	3	0.18
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG21	9	0.18
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG22	9	0.18
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG23	9	0.18
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG21	9	0.18
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG22	9	0.18
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG23	9	0.18
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG21	9	0.18
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG22	9	0.18
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG23	9	0.18
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG21	4	0.18
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG22	4	0.18
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG23	4	0.18
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG21	4	0.18
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG22	4	0.18
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG23	4	0.18
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG21	4	0.18
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG22	4	0.18
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG23	4	0.18
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG11	6	0.18
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG12	6	0.18
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG13	6	0.18
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG11	6	0.18
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG12	6	0.18
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG13	6	0.18
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG11	6	0.18
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG12	6	0.18
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG13	6	0.18
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE1	1	0.18
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE2	1	0.18
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE1	1	0.18
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE2	1	0.18
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE3	1	0.18
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE1	1	0.18
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE2	1	0.18
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE3	1	0.18
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG11	2	0.18
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG12	2	0.18
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG13	2	0.18
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG11	2	0.18
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG12	2	0.18
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG13	2	0.18
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG11	2	0.18
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG12	2	0.18
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG13	2	0.18
(1,436)	1:33:A:ILE:HD11	1:131:A:ILE:HD11	6	0.18
(1,436)	1:33:A:ILE:HD11	1:131:A:ILE:HD12	6	0.18
(1,436)	1:33:A:ILE:HD11	1:131:A:ILE:HD13	6	0.18
(1,436)	1:33:A:ILE:HD12	1:131:A:ILE:HD11	6	0.18
(1,436)	1:33:A:ILE:HD12	1:131:A:ILE:HD12	6	0.18
(1,436)	1:33:A:ILE:HD12	1:131:A:ILE:HD13	6	0.18
(1,436)	1:33:A:ILE:HD13	1:131:A:ILE:HD11	6	0.18
(1,436)	1:33:A:ILE:HD13	1:131:A:ILE:HD12	6	0.18
(1,436)	1:33:A:ILE:HD13	1:131:A:ILE:HD13	6	0.18
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	7	0.18
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	7	0.18
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	7	0.18
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	7	0.18
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	7	0.18
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	7	0.18
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	7	0.18
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	7	0.18
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	7	0.18
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG21	1	0.18
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG22	1	0.18
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG23	1	0.18
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG21	1	0.18
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG22	1	0.18
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG23	1	0.18
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG21	1	0.18
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG22	1	0.18
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG23	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	7	0.18
(1,258)	1:62:A:GLU:H	1:65:A:THR:H	6	0.18
(1,192)	1:104:A:ILE:H	1:106:A:ASN:H	1	0.18
(1,185)	1:83:A:ASN:H	1:85:A:GLN:H	5	0.18
(1,100)	1:167:A:GLY:H	1:168:A:GLY:H	2	0.18
(2,128)	1:60:A:ARG:H	1:56:A:LEU:O	6	0.17
(2,82)	1:28:A:GLN:H	1:24:A:ALA:O	9	0.17
(2,79)	1:190:A:LEU:N	1:87:A:ARG:O	9	0.17
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	6	0.17
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG11	3	0.17
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG12	3	0.17
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG13	3	0.17
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG21	1	0.17
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG22	1	0.17
(1,1088)	1:211:A:SER:H	1:207:A:VAL:HG23	1	0.17
(1,1060)	1:201:A:ARG:H	1:220:A:LEU:HD21	1	0.17
(1,1060)	1:201:A:ARG:H	1:220:A:LEU:HD22	1	0.17
(1,1060)	1:201:A:ARG:H	1:220:A:LEU:HD23	1	0.17
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG21	2	0.17
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG22	2	0.17
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG23	2	0.17
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG21	6	0.17
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG22	6	0.17
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG23	6	0.17
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	6	0.17
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	6	0.17
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	6	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE1	2	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE2	2	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE3	2	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE1	10	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE2	10	0.17
(1,992)	1:185:A:LYS:H	1:98:A:MET:HE3	10	0.17
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB1	1	0.17
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB2	1	0.17
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB3	1	0.17
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG21	7	0.17
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG22	7	0.17
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG23	7	0.17
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	2	0.17
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	2	0.17
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	9	0.17
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	9	0.17
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	9	0.17
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG21	3	0.17
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG22	3	0.17
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG23	3	0.17
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG21	3	0.17
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG22	3	0.17
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG23	3	0.17
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	7	0.17
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	7	0.17
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	7	0.17
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG11	2	0.17
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG12	2	0.17
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG13	2	0.17
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD11	2	0.17
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD12	2	0.17
(1,889)	1:131:A:ILE:H	1:43:A:ILE:HD13	2	0.17
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	8	0.17
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	8	0.17
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	8	0.17
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG21	5	0.17
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG22	5	0.17
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG23	5	0.17
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	3	0.17
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	3	0.17
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	3	0.17
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD11	9	0.17
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD12	9	0.17
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD13	9	0.17
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD21	4	0.17
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD22	4	0.17
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD23	4	0.17
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	9	0.17
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	9	0.17
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	9	0.17
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD11	1	0.17
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD12	1	0.17
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD13	1	0.17
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD11	2	0.17
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD12	2	0.17
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD13	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	8	0.17
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	8	0.17
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	8	0.17
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	4	0.17
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	4	0.17
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	4	0.17
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	3	0.17
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	3	0.17
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	3	0.17
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	6	0.17
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	6	0.17
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	6	0.17
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB1	1	0.17
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB2	1	0.17
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB3	1	0.17
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD11	6	0.17
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD12	6	0.17
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD13	6	0.17
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG21	6	0.17
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG22	6	0.17
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG23	6	0.17
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG21	6	0.17
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG22	6	0.17
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG23	6	0.17
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG21	6	0.17
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG22	6	0.17
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG23	6	0.17
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	9	0.17
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	9	0.17
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	9	0.17
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	9	0.17
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	9	0.17
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	9	0.17
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	9	0.17
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	9	0.17
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	9	0.17
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	10	0.17
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	10	0.17
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	10	0.17
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	10	0.17
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	10	0.17
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	10	0.17
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	10	0.17
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	10	0.17
(1,546)	1:115:A:THR:HG21	1:119:A:MET:HE1	9	0.17
(1,546)	1:115:A:THR:HG21	1:119:A:MET:HE2	9	0.17
(1,546)	1:115:A:THR:HG21	1:119:A:MET:HE3	9	0.17
(1,546)	1:115:A:THR:HG22	1:119:A:MET:HE1	9	0.17
(1,546)	1:115:A:THR:HG22	1:119:A:MET:HE2	9	0.17
(1,546)	1:115:A:THR:HG22	1:119:A:MET:HE3	9	0.17
(1,546)	1:115:A:THR:HG23	1:119:A:MET:HE1	9	0.17
(1,546)	1:115:A:THR:HG23	1:119:A:MET:HE2	9	0.17
(1,546)	1:115:A:THR:HG23	1:119:A:MET:HE3	9	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	1	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	1	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	1	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	1	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	1	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	1	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	1	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	1	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	1	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG21	6	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG22	6	0.17
(1,534)	1:103:A:LEU:HD11	1:172:A:VAL:HG23	6	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG21	6	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG22	6	0.17
(1,534)	1:103:A:LEU:HD12	1:172:A:VAL:HG23	6	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG21	6	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG22	6	0.17
(1,534)	1:103:A:LEU:HD13	1:172:A:VAL:HG23	6	0.17
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	3	0.17
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	3	0.17
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	3	0.17
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	3	0.17
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	3	0.17
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	3	0.17
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	3	0.17
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	3	0.17
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	3	0.17
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	6	0.17
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	6	0.17
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	6	0.17
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	6	0.17
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	6	0.17
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	6	0.17
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	6	0.17
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	6	0.17
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	4	0.17
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	4	0.17
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	4	0.17
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	4	0.17
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	4	0.17
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	4	0.17
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	4	0.17
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	4	0.17
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	4	0.17
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	9	0.17
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	9	0.17
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	9	0.17
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	9	0.17
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	9	0.17
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	9	0.17
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	9	0.17
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	9	0.17
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	9	0.17
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	8	0.17
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	8	0.17
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	8	0.17
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	8	0.17
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	8	0.17
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	8	0.17
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	8	0.17
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	8	0.17
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	8	0.17
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	1	0.17
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	1	0.17
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	1	0.17
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	1	0.17
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	1	0.17
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	1	0.17
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	1	0.17
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	1	0.17
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG21	2	0.17
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG22	2	0.17
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG23	2	0.17
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG21	2	0.17
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG22	2	0.17
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG23	2	0.17
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG21	2	0.17
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG22	2	0.17
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG23	2	0.17
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD11	8	0.17
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD12	8	0.17
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD13	8	0.17
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD11	8	0.17
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD12	8	0.17
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD13	8	0.17
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD11	8	0.17
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD12	8	0.17
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD13	8	0.17
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD11	10	0.17
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD12	10	0.17
(1,459)	1:45:A:LEU:HD21	1:188:A:LEU:HD13	10	0.17
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD11	10	0.17
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD12	10	0.17
(1,459)	1:45:A:LEU:HD22	1:188:A:LEU:HD13	10	0.17
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD11	10	0.17
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD12	10	0.17
(1,459)	1:45:A:LEU:HD23	1:188:A:LEU:HD13	10	0.17
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	4	0.17
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	4	0.17
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	4	0.17
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	4	0.17
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	4	0.17
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	4	0.17
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	4	0.17
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	4	0.17
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	4	0.17
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG21	7	0.17
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG22	7	0.17
(1,409)	1:26:A:ILE:HD11	1:136:A:VAL:HG23	7	0.17
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG21	7	0.17
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG22	7	0.17
(1,409)	1:26:A:ILE:HD12	1:136:A:VAL:HG23	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG21	7	0.17
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG22	7	0.17
(1,409)	1:26:A:ILE:HD13	1:136:A:VAL:HG23	7	0.17
(1,374)	1:225:A:GLU:H	1:230:A:VAL:H	10	0.17
(1,349)	1:147:A:LYS:H	1:189:A:HIS:H	2	0.17
(1,341)	1:95:A:GLY:H	1:184:A:THR:H	5	0.17
(1,314)	1:58:A:LYS:H	1:96:A:ILE:H	7	0.17
(1,312)	1:56:A:LEU:H	1:96:A:ILE:H	8	0.17
(1,311)	1:55:A:ALA:H	1:96:A:ILE:H	4	0.17
(1,278)	1:131:A:ILE:H	1:134:A:PHE:H	4	0.17
(1,247)	1:35:A:ASN:H	1:38:A:TYR:H	1	0.17
(1,208)	1:136:A:VAL:H	1:138:A:PHE:H	2	0.17
(1,192)	1:104:A:ILE:H	1:106:A:ASN:H	6	0.17
(1,182)	1:70:A:LEU:H	1:72:A:SER:H	9	0.17
(1,180)	1:68:A:SER:H	1:70:A:LEU:H	5	0.17
(1,107)	1:176:A:THR:H	1:177:A:GLY:H	3	0.17
(1,107)	1:176:A:THR:H	1:177:A:GLY:H	10	0.17
(1,73)	1:127:A:ASP:H	1:128:A:ILE:H	5	0.17
(2,148)	1:210:A:HIS:H	1:206:A:ILE:O	8	0.16
(2,132)	1:62:A:GLU:H	1:58:A:LYS:O	4	0.16
(2,80)	1:190:A:LEU:H	1:87:A:ARG:O	6	0.16
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG11	2	0.16
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG12	2	0.16
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG13	2	0.16
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG21	4	0.16
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG22	4	0.16
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG23	4	0.16
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	2	0.16
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	2	0.16
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	2	0.16
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG11	1	0.16
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG12	1	0.16
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG13	1	0.16
(1,1017)	1:188:A:LEU:H	1:145:A:ALA:HB1	7	0.16
(1,1017)	1:188:A:LEU:H	1:145:A:ALA:HB2	7	0.16
(1,1017)	1:188:A:LEU:H	1:145:A:ALA:HB3	7	0.16
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	5	0.16
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	5	0.16
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	5	0.16
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	6	0.16
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	6	0.16
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG21	1	0.16
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG22	1	0.16
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG23	1	0.16
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	6	0.16
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	6	0.16
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	6	0.16
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	9	0.16
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	9	0.16
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	9	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG11	9	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG12	9	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG13	9	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG11	10	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG12	10	0.16
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG13	10	0.16
(1,906)	1:141:A:ALA:H	1:131:A:ILE:HD11	7	0.16
(1,906)	1:141:A:ALA:H	1:131:A:ILE:HD12	7	0.16
(1,906)	1:141:A:ALA:H	1:131:A:ILE:HD13	7	0.16
(1,903)	1:139:A:TYR:H	1:131:A:ILE:HD11	5	0.16
(1,903)	1:139:A:TYR:H	1:131:A:ILE:HD12	5	0.16
(1,903)	1:139:A:TYR:H	1:131:A:ILE:HD13	5	0.16
(1,902)	1:139:A:TYR:H	1:48:A:LEU:HD11	2	0.16
(1,902)	1:139:A:TYR:H	1:48:A:LEU:HD12	2	0.16
(1,902)	1:139:A:TYR:H	1:48:A:LEU:HD13	2	0.16
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG21	3	0.16
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG22	3	0.16
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG23	3	0.16
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG21	5	0.16
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG22	5	0.16
(1,897)	1:138:A:PHE:H	1:109:A:THR:HG23	5	0.16
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	2	0.16
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	2	0.16
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	2	0.16
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE1	3	0.16
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE2	3	0.16
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE3	3	0.16
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	9	0.16
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	9	0.16
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	9	0.16
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	2	0.16
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	2	0.16
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	6	0.16
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	6	0.16
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	6	0.16
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	3	0.16
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	3	0.16
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	3	0.16
(1,825)	1:89:A:LEU:H	1:188:A:LEU:HD21	3	0.16
(1,825)	1:89:A:LEU:H	1:188:A:LEU:HD22	3	0.16
(1,825)	1:89:A:LEU:H	1:188:A:LEU:HD23	3	0.16
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG21	10	0.16
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG22	10	0.16
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG23	10	0.16
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG21	5	0.16
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG22	5	0.16
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG23	5	0.16
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD21	2	0.16
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD22	2	0.16
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD23	2	0.16
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD11	9	0.16
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD12	9	0.16
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD13	9	0.16
(1,779)	1:74:A:LYS:H	1:94:A:THR:HG21	5	0.16
(1,779)	1:74:A:LYS:H	1:94:A:THR:HG22	5	0.16
(1,779)	1:74:A:LYS:H	1:94:A:THR:HG23	5	0.16
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD21	4	0.16
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD22	4	0.16
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD23	4	0.16
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	9	0.16
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	9	0.16
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	9	0.16
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	3	0.16
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	3	0.16
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	3	0.16
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB1	9	0.16
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB2	9	0.16
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB3	9	0.16
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG21	4	0.16
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG22	4	0.16
(1,694)	1:26:A:ILE:H	1:115:A:THR:HG23	4	0.16
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB1	9	0.16
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB2	9	0.16
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	9	0.16
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	9	0.16
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	9	0.16
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG11	1	0.16
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG12	1	0.16
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG13	1	0.16
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG11	2	0.16
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG12	2	0.16
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG13	2	0.16
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG11	6	0.16
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG12	6	0.16
(1,684)	1:18:A:GLU:H	1:172:A:VAL:HG13	6	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG21	8	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG22	8	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG23	8	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG21	10	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG22	10	0.16
(1,683)	1:18:A:GLU:H	1:17:A:VAL:HG23	10	0.16
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	1	0.16
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	1	0.16
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	1	0.16
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	7	0.16
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	7	0.16
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	7	0.16
(1,627)	1:76:A:LEU:H	1:76:A:LEU:HD11	3	0.16
(1,627)	1:76:A:LEU:H	1:76:A:LEU:HD12	3	0.16
(1,627)	1:76:A:LEU:H	1:76:A:LEU:HD13	3	0.16
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD11	2	0.16
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD12	2	0.16
(1,601)	1:207:A:VAL:HG21	1:218:A:ILE:HD13	2	0.16
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD11	2	0.16
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD12	2	0.16
(1,601)	1:207:A:VAL:HG22	1:218:A:ILE:HD13	2	0.16
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD11	2	0.16
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD12	2	0.16
(1,601)	1:207:A:VAL:HG23	1:218:A:ILE:HD13	2	0.16
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD21	8	0.16
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD22	8	0.16
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD23	8	0.16
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD21	8	0.16
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD22	8	0.16
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD23	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD21	8	0.16
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD22	8	0.16
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD23	8	0.16
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD11	10	0.16
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD12	10	0.16
(1,576)	1:149:A:THR:HG21	1:187:A:ILE:HD13	10	0.16
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD11	10	0.16
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD12	10	0.16
(1,576)	1:149:A:THR:HG22	1:187:A:ILE:HD13	10	0.16
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD11	10	0.16
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD12	10	0.16
(1,576)	1:149:A:THR:HG23	1:187:A:ILE:HD13	10	0.16
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	8	0.16
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	8	0.16
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	8	0.16
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	8	0.16
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	8	0.16
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	8	0.16
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	8	0.16
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	8	0.16
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	8	0.16
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	7	0.16
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	7	0.16
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	7	0.16
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	7	0.16
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	7	0.16
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	7	0.16
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	7	0.16
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	7	0.16
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	7	0.16
(1,541)	1:104:A:ILE:HD11	1:172:A:VAL:HG21	1	0.16
(1,541)	1:104:A:ILE:HD11	1:172:A:VAL:HG22	1	0.16
(1,541)	1:104:A:ILE:HD11	1:172:A:VAL:HG23	1	0.16
(1,541)	1:104:A:ILE:HD12	1:172:A:VAL:HG21	1	0.16
(1,541)	1:104:A:ILE:HD12	1:172:A:VAL:HG22	1	0.16
(1,541)	1:104:A:ILE:HD12	1:172:A:VAL:HG23	1	0.16
(1,541)	1:104:A:ILE:HD13	1:172:A:VAL:HG21	1	0.16
(1,541)	1:104:A:ILE:HD13	1:172:A:VAL:HG22	1	0.16
(1,541)	1:104:A:ILE:HD13	1:172:A:VAL:HG23	1	0.16
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	8	0.16
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	8	0.16
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	8	0.16
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	8	0.16
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	8	0.16
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	8	0.16
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	8	0.16
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	8	0.16
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	4	0.16
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	4	0.16
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	4	0.16
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	4	0.16
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	4	0.16
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	4	0.16
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	4	0.16
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	4	0.16
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	4	0.16
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	5	0.16
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	5	0.16
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	5	0.16
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	5	0.16
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	5	0.16
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	5	0.16
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	5	0.16
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	5	0.16
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	5	0.16
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG11	7	0.16
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG12	7	0.16
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG13	7	0.16
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG11	7	0.16
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG12	7	0.16
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG13	7	0.16
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG11	7	0.16
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG12	7	0.16
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG13	7	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	1	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	1	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	1	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	1	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	1	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	1	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	1	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	1	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	9	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	9	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	9	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	9	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	9	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	9	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	9	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	9	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	9	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	10	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	10	0.16
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	10	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	10	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	10	0.16
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	10	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	10	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	10	0.16
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	10	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	6	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	6	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	6	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	6	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	6	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	6	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	6	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	6	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	6	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	10	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	10	0.16
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	10	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	10	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	10	0.16
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	10	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	10	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	10	0.16
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	10	0.16
(1,417)	1:29:A:LEU:HD11	1:131:A:ILE:HD11	10	0.16
(1,417)	1:29:A:LEU:HD11	1:131:A:ILE:HD12	10	0.16
(1,417)	1:29:A:LEU:HD11	1:131:A:ILE:HD13	10	0.16
(1,417)	1:29:A:LEU:HD12	1:131:A:ILE:HD11	10	0.16
(1,417)	1:29:A:LEU:HD12	1:131:A:ILE:HD12	10	0.16
(1,417)	1:29:A:LEU:HD12	1:131:A:ILE:HD13	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:29:A:LEU:HD13	1:131:A:ILE:HD11	10	0.16
(1,417)	1:29:A:LEU:HD13	1:131:A:ILE:HD12	10	0.16
(1,417)	1:29:A:LEU:HD13	1:131:A:ILE:HD13	10	0.16
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	10	0.16
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	10	0.16
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	10	0.16
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	10	0.16
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	10	0.16
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	10	0.16
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	10	0.16
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	10	0.16
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	10	0.16
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB1	9	0.16
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB2	9	0.16
(1,407)	1:26:A:ILE:HD11	1:111:A:ALA:HB3	9	0.16
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB1	9	0.16
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB2	9	0.16
(1,407)	1:26:A:ILE:HD12	1:111:A:ALA:HB3	9	0.16
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB1	9	0.16
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB2	9	0.16
(1,407)	1:26:A:ILE:HD13	1:111:A:ALA:HB3	9	0.16
(1,404)	1:17:A:VAL:HG11	1:171:A:THR:HG21	9	0.16
(1,404)	1:17:A:VAL:HG11	1:171:A:THR:HG22	9	0.16
(1,404)	1:17:A:VAL:HG11	1:171:A:THR:HG23	9	0.16
(1,404)	1:17:A:VAL:HG12	1:171:A:THR:HG21	9	0.16
(1,404)	1:17:A:VAL:HG12	1:171:A:THR:HG22	9	0.16
(1,404)	1:17:A:VAL:HG12	1:171:A:THR:HG23	9	0.16
(1,404)	1:17:A:VAL:HG13	1:171:A:THR:HG21	9	0.16
(1,404)	1:17:A:VAL:HG13	1:171:A:THR:HG22	9	0.16
(1,404)	1:17:A:VAL:HG13	1:171:A:THR:HG23	9	0.16
(1,373)	1:210:A:HIS:H	1:214:A:ILE:H	9	0.16
(1,260)	1:66:A:ASP:H	1:69:A:LYS:H	1	0.16
(1,243)	1:224:A:LYS:H	1:226:A:ARG:H	4	0.16
(1,189)	1:95:A:GLY:H	1:97:A:GLY:H	9	0.16
(1,63)	1:105:A:ASN:H	1:106:A:ASN:H	1	0.16
(1,63)	1:105:A:ASN:H	1:106:A:ASN:H	6	0.16
(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	2	0.15
(2,12)	1:78:A:ILE:H	1:217:A:PRO:O	2	0.15
(1,1117)	1:123:A:GLN:HE21	1:119:A:MET:HE1	9	0.15
(1,1117)	1:123:A:GLN:HE21	1:119:A:MET:HE2	9	0.15
(1,1117)	1:123:A:GLN:HE21	1:119:A:MET:HE3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG11	3	0.15
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG12	3	0.15
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG13	3	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG21	2	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG22	2	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG23	2	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG21	6	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG22	6	0.15
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG23	6	0.15
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD11	2	0.15
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD12	2	0.15
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD13	2	0.15
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG21	8	0.15
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG22	8	0.15
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG23	8	0.15
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	8	0.15
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	8	0.15
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	8	0.15
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	8	0.15
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	8	0.15
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	8	0.15
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	4	0.15
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	4	0.15
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	4	0.15
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG21	9	0.15
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG22	9	0.15
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG23	9	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG21	2	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG22	2	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG23	2	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG21	4	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG22	4	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG23	4	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG21	8	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG22	8	0.15
(1,1028)	1:190:A:LEU:H	1:88:A:THR:HG23	8	0.15
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG11	4	0.15
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG12	4	0.15
(1,1007)	1:187:A:ILE:H	1:150:A:VAL:HG13	4	0.15
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG21	1	0.15
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG22	1	0.15
(1,1002)	1:186:A:VAL:H	1:150:A:VAL:HG23	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:186:A:VAL:H	1:150:A:VAL:HG11	1	0.15
(1,1001)	1:186:A:VAL:H	1:150:A:VAL:HG12	1	0.15
(1,1001)	1:186:A:VAL:H	1:150:A:VAL:HG13	1	0.15
(1,991)	1:185:A:LYS:H	1:92:A:VAL:HG21	4	0.15
(1,991)	1:185:A:LYS:H	1:92:A:VAL:HG22	4	0.15
(1,991)	1:185:A:LYS:H	1:92:A:VAL:HG23	4	0.15
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	8	0.15
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	8	0.15
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	8	0.15
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD21	5	0.15
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD22	5	0.15
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD23	5	0.15
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG21	4	0.15
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG22	4	0.15
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG23	4	0.15
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	2	0.15
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	2	0.15
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	2	0.15
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG21	4	0.15
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG22	4	0.15
(1,961)	1:162:A:TRP:H	1:150:A:VAL:HG23	4	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG21	4	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG22	4	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG23	4	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG21	7	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG22	7	0.15
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG23	7	0.15
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG21	10	0.15
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG22	10	0.15
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG23	10	0.15
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG11	3	0.15
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG12	3	0.15
(1,932)	1:149:A:THR:H	1:148:A:VAL:HG13	3	0.15
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	8	0.15
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	8	0.15
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	8	0.15
(1,901)	1:139:A:TYR:H	1:33:A:ILE:HD11	3	0.15
(1,901)	1:139:A:TYR:H	1:33:A:ILE:HD12	3	0.15
(1,901)	1:139:A:TYR:H	1:33:A:ILE:HD13	3	0.15
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	10	0.15
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	10	0.15
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB1	8	0.15
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB2	8	0.15
(1,879)	1:126:A:ALA:H	1:121:A:ALA:HB3	8	0.15
(1,873)	1:123:A:GLN:H	1:122:A:LEU:HD11	7	0.15
(1,873)	1:123:A:GLN:H	1:122:A:LEU:HD12	7	0.15
(1,873)	1:123:A:GLN:H	1:122:A:LEU:HD13	7	0.15
(1,862)	1:111:A:ALA:H	1:109:A:THR:HG21	2	0.15
(1,862)	1:111:A:ALA:H	1:109:A:THR:HG22	2	0.15
(1,862)	1:111:A:ALA:H	1:109:A:THR:HG23	2	0.15
(1,861)	1:111:A:ALA:H	1:26:A:ILE:HD11	1	0.15
(1,861)	1:111:A:ALA:H	1:26:A:ILE:HD12	1	0.15
(1,861)	1:111:A:ALA:H	1:26:A:ILE:HD13	1	0.15
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD11	1	0.15
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD12	1	0.15
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD13	1	0.15
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	7	0.15
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	7	0.15
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	7	0.15
(1,848)	1:96:A:ILE:H	1:55:A:ALA:HB1	7	0.15
(1,848)	1:96:A:ILE:H	1:55:A:ALA:HB2	7	0.15
(1,848)	1:96:A:ILE:H	1:55:A:ALA:HB3	7	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD11	5	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD12	5	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD13	5	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD11	9	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD12	9	0.15
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD13	9	0.15
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	8	0.15
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	8	0.15
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	8	0.15
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	9	0.15
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	9	0.15
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	9	0.15
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD11	2	0.15
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD12	2	0.15
(1,824)	1:89:A:LEU:H	1:188:A:LEU:HD13	2	0.15
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG21	10	0.15
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG22	10	0.15
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG23	10	0.15
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG21	4	0.15
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG22	4	0.15
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG23	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD11	5	0.15
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD12	5	0.15
(1,774)	1:70:A:LEU:H	1:59:A:ILE:HD13	5	0.15
(1,769)	1:66:A:ASP:H	1:64:A:LEU:HD11	6	0.15
(1,769)	1:66:A:ASP:H	1:64:A:LEU:HD12	6	0.15
(1,769)	1:66:A:ASP:H	1:64:A:LEU:HD13	6	0.15
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD11	3	0.15
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD12	3	0.15
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD13	3	0.15
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	4	0.15
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	4	0.15
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	4	0.15
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD11	4	0.15
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD12	4	0.15
(1,720)	1:43:A:ILE:H	1:143:A:LEU:HD13	4	0.15
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG11	1	0.15
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG12	1	0.15
(1,719)	1:42:A:GLU:H	1:144:A:VAL:HG13	1	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	1	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	1	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	1	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	9	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	9	0.15
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	9	0.15
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	5	0.15
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	5	0.15
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	5	0.15
(1,702)	1:31:A:SER:H	1:30:A:MET:HE1	2	0.15
(1,702)	1:31:A:SER:H	1:30:A:MET:HE2	2	0.15
(1,702)	1:31:A:SER:H	1:30:A:MET:HE3	2	0.15
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB1	2	0.15
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB2	2	0.15
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB3	2	0.15
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB1	8	0.15
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB2	8	0.15
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB3	8	0.15
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG21	1	0.15
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG22	1	0.15
(1,690)	1:21:A:ALA:H	1:109:A:THR:HG23	1	0.15
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG21	9	0.15
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG22	9	0.15
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG23	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	7	0.15
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	7	0.15
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	7	0.15
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG11	3	0.15
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG12	3	0.15
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG13	3	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	5	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	5	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	5	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	6	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	6	0.15
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	6	0.15
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD21	1	0.15
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD22	1	0.15
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD23	1	0.15
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD11	5	0.15
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD12	5	0.15
(1,622)	1:59:A:ILE:H	1:59:A:ILE:HD13	5	0.15
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD11	4	0.15
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD12	4	0.15
(1,596)	1:195:A:THR:HG21	1:198:A:LEU:HD13	4	0.15
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD11	4	0.15
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD12	4	0.15
(1,596)	1:195:A:THR:HG22	1:198:A:LEU:HD13	4	0.15
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD11	4	0.15
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD12	4	0.15
(1,596)	1:195:A:THR:HG23	1:198:A:LEU:HD13	4	0.15
(1,594)	1:190:A:LEU:HD21	1:198:A:LEU:HD11	8	0.15
(1,594)	1:190:A:LEU:HD21	1:198:A:LEU:HD12	8	0.15
(1,594)	1:190:A:LEU:HD21	1:198:A:LEU:HD13	8	0.15
(1,594)	1:190:A:LEU:HD22	1:198:A:LEU:HD11	8	0.15
(1,594)	1:190:A:LEU:HD22	1:198:A:LEU:HD12	8	0.15
(1,594)	1:190:A:LEU:HD22	1:198:A:LEU:HD13	8	0.15
(1,594)	1:190:A:LEU:HD23	1:198:A:LEU:HD11	8	0.15
(1,594)	1:190:A:LEU:HD23	1:198:A:LEU:HD12	8	0.15
(1,594)	1:190:A:LEU:HD23	1:198:A:LEU:HD13	8	0.15
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD11	6	0.15
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD12	6	0.15
(1,563)	1:141:A:ALA:HB1	1:188:A:LEU:HD13	6	0.15
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD11	6	0.15
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD12	6	0.15
(1,563)	1:141:A:ALA:HB2	1:188:A:LEU:HD13	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD11	6	0.15
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD12	6	0.15
(1,563)	1:141:A:ALA:HB3	1:188:A:LEU:HD13	6	0.15
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG21	3	0.15
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG22	3	0.15
(1,561)	1:141:A:ALA:HB1	1:148:A:VAL:HG23	3	0.15
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG21	3	0.15
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG22	3	0.15
(1,561)	1:141:A:ALA:HB2	1:148:A:VAL:HG23	3	0.15
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG21	3	0.15
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG22	3	0.15
(1,561)	1:141:A:ALA:HB3	1:148:A:VAL:HG23	3	0.15
(1,557)	1:128:A:ILE:HD11	1:143:A:LEU:HD11	8	0.15
(1,557)	1:128:A:ILE:HD11	1:143:A:LEU:HD12	8	0.15
(1,557)	1:128:A:ILE:HD11	1:143:A:LEU:HD13	8	0.15
(1,557)	1:128:A:ILE:HD12	1:143:A:LEU:HD11	8	0.15
(1,557)	1:128:A:ILE:HD12	1:143:A:LEU:HD12	8	0.15
(1,557)	1:128:A:ILE:HD12	1:143:A:LEU:HD13	8	0.15
(1,557)	1:128:A:ILE:HD13	1:143:A:LEU:HD11	8	0.15
(1,557)	1:128:A:ILE:HD13	1:143:A:LEU:HD12	8	0.15
(1,557)	1:128:A:ILE:HD13	1:143:A:LEU:HD13	8	0.15
(1,554)	1:122:A:LEU:HD11	1:128:A:ILE:HD11	9	0.15
(1,554)	1:122:A:LEU:HD11	1:128:A:ILE:HD12	9	0.15
(1,554)	1:122:A:LEU:HD11	1:128:A:ILE:HD13	9	0.15
(1,554)	1:122:A:LEU:HD12	1:128:A:ILE:HD11	9	0.15
(1,554)	1:122:A:LEU:HD12	1:128:A:ILE:HD12	9	0.15
(1,554)	1:122:A:LEU:HD12	1:128:A:ILE:HD13	9	0.15
(1,554)	1:122:A:LEU:HD13	1:128:A:ILE:HD11	9	0.15
(1,554)	1:122:A:LEU:HD13	1:128:A:ILE:HD12	9	0.15
(1,554)	1:122:A:LEU:HD13	1:128:A:ILE:HD13	9	0.15
(1,538)	1:103:A:LEU:HD21	1:172:A:VAL:HG11	2	0.15
(1,538)	1:103:A:LEU:HD21	1:172:A:VAL:HG12	2	0.15
(1,538)	1:103:A:LEU:HD21	1:172:A:VAL:HG13	2	0.15
(1,538)	1:103:A:LEU:HD22	1:172:A:VAL:HG11	2	0.15
(1,538)	1:103:A:LEU:HD22	1:172:A:VAL:HG12	2	0.15
(1,538)	1:103:A:LEU:HD22	1:172:A:VAL:HG13	2	0.15
(1,538)	1:103:A:LEU:HD23	1:172:A:VAL:HG11	2	0.15
(1,538)	1:103:A:LEU:HD23	1:172:A:VAL:HG12	2	0.15
(1,538)	1:103:A:LEU:HD23	1:172:A:VAL:HG13	2	0.15
(1,537)	1:103:A:LEU:HD21	1:152:A:THR:HG21	6	0.15
(1,537)	1:103:A:LEU:HD21	1:152:A:THR:HG22	6	0.15
(1,537)	1:103:A:LEU:HD21	1:152:A:THR:HG23	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:103:A:LEU:HD22	1:152:A:THR:HG21	6	0.15
(1,537)	1:103:A:LEU:HD22	1:152:A:THR:HG22	6	0.15
(1,537)	1:103:A:LEU:HD22	1:152:A:THR:HG23	6	0.15
(1,537)	1:103:A:LEU:HD23	1:152:A:THR:HG21	6	0.15
(1,537)	1:103:A:LEU:HD23	1:152:A:THR:HG22	6	0.15
(1,537)	1:103:A:LEU:HD23	1:152:A:THR:HG23	6	0.15
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	5	0.15
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	5	0.15
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	5	0.15
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	5	0.15
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	5	0.15
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	5	0.15
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	5	0.15
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	5	0.15
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	5	0.15
(1,522)	1:98:A:MET:HE1	1:107:A:LEU:HD21	9	0.15
(1,522)	1:98:A:MET:HE1	1:107:A:LEU:HD22	9	0.15
(1,522)	1:98:A:MET:HE1	1:107:A:LEU:HD23	9	0.15
(1,522)	1:98:A:MET:HE2	1:107:A:LEU:HD21	9	0.15
(1,522)	1:98:A:MET:HE2	1:107:A:LEU:HD22	9	0.15
(1,522)	1:98:A:MET:HE2	1:107:A:LEU:HD23	9	0.15
(1,522)	1:98:A:MET:HE3	1:107:A:LEU:HD21	9	0.15
(1,522)	1:98:A:MET:HE3	1:107:A:LEU:HD22	9	0.15
(1,522)	1:98:A:MET:HE3	1:107:A:LEU:HD23	9	0.15
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE1	9	0.15
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE2	9	0.15
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE3	9	0.15
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE1	9	0.15
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE2	9	0.15
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE3	9	0.15
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE1	9	0.15
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE2	9	0.15
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE3	9	0.15
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD11	3	0.15
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD12	3	0.15
(1,513)	1:91:A:ILE:HD11	1:188:A:LEU:HD13	3	0.15
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD11	3	0.15
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD12	3	0.15
(1,513)	1:91:A:ILE:HD12	1:188:A:LEU:HD13	3	0.15
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD11	3	0.15
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD12	3	0.15
(1,513)	1:91:A:ILE:HD13	1:188:A:LEU:HD13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD11	6	0.15
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD12	6	0.15
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD13	6	0.15
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD11	6	0.15
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD12	6	0.15
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD13	6	0.15
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD11	6	0.15
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD12	6	0.15
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD13	6	0.15
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	3	0.15
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	3	0.15
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	3	0.15
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	3	0.15
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	3	0.15
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	3	0.15
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	3	0.15
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	3	0.15
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	3	0.15
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	2	0.15
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	2	0.15
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	2	0.15
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	2	0.15
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	2	0.15
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	2	0.15
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	2	0.15
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	2	0.15
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	2	0.15
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	4	0.15
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	4	0.15
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	4	0.15
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	4	0.15
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	4	0.15
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	4	0.15
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	4	0.15
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	4	0.15
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	4	0.15
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	7	0.15
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	7	0.15
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	7	0.15
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	7	0.15
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	7	0.15
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	7	0.15
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	7	0.15
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	7	0.15
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	5	0.15
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	5	0.15
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	5	0.15
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	5	0.15
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	5	0.15
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	5	0.15
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	5	0.15
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	5	0.15
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	5	0.15
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG21	9	0.15
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG22	9	0.15
(1,485)	1:64:A:LEU:HD11	1:65:A:THR:HG23	9	0.15
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG21	9	0.15
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG22	9	0.15
(1,485)	1:64:A:LEU:HD12	1:65:A:THR:HG23	9	0.15
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG21	9	0.15
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG22	9	0.15
(1,485)	1:64:A:LEU:HD13	1:65:A:THR:HG23	9	0.15
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	2	0.15
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	2	0.15
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	2	0.15
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	2	0.15
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	2	0.15
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	2	0.15
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	2	0.15
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	2	0.15
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	2	0.15
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	9	0.15
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	9	0.15
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	9	0.15
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	9	0.15
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	9	0.15
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	9	0.15
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	9	0.15
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	9	0.15
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	9	0.15
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB1	5	0.15
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB2	5	0.15
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB1	5	0.15
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB2	5	0.15
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB3	5	0.15
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB1	5	0.15
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB2	5	0.15
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB3	5	0.15
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	5	0.15
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	10	0.15
(1,283)	1:142:A:TYR:H	1:145:A:ALA:H	3	0.15
(1,282)	1:138:A:PHE:H	1:141:A:ALA:H	8	0.15
(1,267)	1:99:A:THR:H	1:102:A:ASP:H	10	0.15
(1,259)	1:63:A:SER:H	1:66:A:ASP:H	3	0.15
(1,57)	1:96:A:ILE:H	1:97:A:GLY:H	1	0.15
(1,57)	1:96:A:ILE:H	1:97:A:GLY:H	10	0.15
(1,47)	1:84:A:LYS:H	1:85:A:GLN:H	5	0.15
(1,34)	1:68:A:SER:H	1:69:A:LYS:H	9	0.15
(2,148)	1:210:A:HIS:H	1:206:A:ILE:O	4	0.14
(2,68)	1:153:A:LYS:H	1:183:A:GLY:O	10	0.14
(2,66)	1:160:A:TYR:H	1:152:A:THR:O	10	0.14
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	3	0.14
(2,43)	1:147:A:LYS:N	1:189:A:HIS:O	4	0.14
(2,30)	1:88:A:THR:H	1:83:A:ASN:O	4	0.14
(2,22)	1:221:A:PHE:H	1:80:A:LEU:O	9	0.14
(2,16)	1:79:A:ASN:H	1:92:A:VAL:O	2	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD11	6	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD12	6	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD13	6	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD11	10	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD12	10	0.14
(1,1094)	1:216:A:TYR:H	1:78:A:ILE:HD13	10	0.14
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG21	7	0.14
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG22	7	0.14
(1,1089)	1:212:A:GLN:H	1:207:A:VAL:HG23	7	0.14
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD11	4	0.14
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD12	4	0.14
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD13	4	0.14
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD11	8	0.14
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD12	8	0.14
(1,1063)	1:203:A:ILE:H	1:206:A:ILE:HD13	8	0.14
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG21	1	0.14
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG22	1	0.14
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG23	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD11	4	0.14
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD12	4	0.14
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD13	4	0.14
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD21	6	0.14
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD22	6	0.14
(1,1045)	1:197:A:TYR:H	1:190:A:LEU:HD23	6	0.14
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG11	1	0.14
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG12	1	0.14
(1,993)	1:185:A:LYS:H	1:150:A:VAL:HG13	1	0.14
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD21	9	0.14
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD22	9	0.14
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD23	9	0.14
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG21	6	0.14
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG22	6	0.14
(1,976)	1:172:A:VAL:H	1:17:A:VAL:HG23	6	0.14
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG21	1	0.14
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG22	1	0.14
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG23	1	0.14
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	6	0.14
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	6	0.14
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	6	0.14
(1,948)	1:152:A:THR:H	1:184:A:THR:HG21	2	0.14
(1,948)	1:152:A:THR:H	1:184:A:THR:HG22	2	0.14
(1,948)	1:152:A:THR:H	1:184:A:THR:HG23	2	0.14
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG21	1	0.14
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG22	1	0.14
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG23	1	0.14
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG21	2	0.14
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG22	2	0.14
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG23	2	0.14
(1,935)	1:150:A:VAL:H	1:148:A:VAL:HG11	2	0.14
(1,935)	1:150:A:VAL:H	1:148:A:VAL:HG12	2	0.14
(1,935)	1:150:A:VAL:H	1:148:A:VAL:HG13	2	0.14
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG11	6	0.14
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG12	6	0.14
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG13	6	0.14
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB1	7	0.14
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB2	7	0.14
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB3	7	0.14
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD11	4	0.14
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD12	4	0.14
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD13	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD11	9	0.14
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD12	9	0.14
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD13	9	0.14
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	10	0.14
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	10	0.14
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	10	0.14
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD21	4	0.14
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD22	4	0.14
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD23	4	0.14
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	5	0.14
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	5	0.14
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	5	0.14
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD21	10	0.14
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD22	10	0.14
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD23	10	0.14
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG11	7	0.14
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG12	7	0.14
(1,794)	1:79:A:ASN:H	1:92:A:VAL:HG13	7	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD21	1	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD22	1	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD23	1	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD21	7	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD22	7	0.14
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD23	7	0.14
(1,790)	1:79:A:ASN:H	1:78:A:ILE:HD11	2	0.14
(1,790)	1:79:A:ASN:H	1:78:A:ILE:HD12	2	0.14
(1,790)	1:79:A:ASN:H	1:78:A:ILE:HD13	2	0.14
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG21	6	0.14
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG22	6	0.14
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG23	6	0.14
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD11	6	0.14
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD12	6	0.14
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD13	6	0.14
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD11	8	0.14
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD12	8	0.14
(1,780)	1:75:A:GLU:H	1:70:A:LEU:HD13	8	0.14
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD11	3	0.14
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD12	3	0.14
(1,771)	1:69:A:LYS:H	1:59:A:ILE:HD13	3	0.14
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	6	0.14
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	6	0.14
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB1	9	0.14
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB2	9	0.14
(1,745)	1:56:A:LEU:H	1:55:A:ALA:HB3	9	0.14
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD11	5	0.14
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD12	5	0.14
(1,714)	1:34:A:ILE:H	1:33:A:ILE:HD13	5	0.14
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	6	0.14
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	6	0.14
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	6	0.14
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	4	0.14
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	4	0.14
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	4	0.14
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	8	0.14
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	8	0.14
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	8	0.14
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	1	0.14
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	1	0.14
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	1	0.14
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	1	0.14
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	1	0.14
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	1	0.14
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	1	0.14
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	1	0.14
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	1	0.14
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD21	2	0.14
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD22	2	0.14
(1,597)	1:195:A:THR:HG21	1:198:A:LEU:HD23	2	0.14
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD21	2	0.14
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD22	2	0.14
(1,597)	1:195:A:THR:HG22	1:198:A:LEU:HD23	2	0.14
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD21	2	0.14
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD22	2	0.14
(1,597)	1:195:A:THR:HG23	1:198:A:LEU:HD23	2	0.14
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG21	3	0.14
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG22	3	0.14
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG23	3	0.14
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG21	3	0.14
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG22	3	0.14
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG23	3	0.14
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG21	3	0.14
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG22	3	0.14
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG23	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB1	6	0.14
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB2	6	0.14
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB3	6	0.14
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB1	6	0.14
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB2	6	0.14
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB3	6	0.14
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB1	6	0.14
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB2	6	0.14
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB3	6	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	7	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	7	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	7	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	7	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	7	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	7	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	7	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	7	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	7	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	9	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	9	0.14
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	9	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	9	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	9	0.14
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	9	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	9	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	9	0.14
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	9	0.14
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE1	4	0.14
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE2	4	0.14
(1,556)	1:126:A:ALA:HB1	1:130:A:MET:HE3	4	0.14
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE1	4	0.14
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE2	4	0.14
(1,556)	1:126:A:ALA:HB2	1:130:A:MET:HE3	4	0.14
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE1	4	0.14
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE2	4	0.14
(1,556)	1:126:A:ALA:HB3	1:130:A:MET:HE3	4	0.14
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB1	5	0.14
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB2	5	0.14
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB3	5	0.14
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB1	5	0.14
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB2	5	0.14
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB1	5	0.14
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB2	5	0.14
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB3	5	0.14
(1,552)	1:121:A:ALA:HB1	1:130:A:MET:HE1	1	0.14
(1,552)	1:121:A:ALA:HB1	1:130:A:MET:HE2	1	0.14
(1,552)	1:121:A:ALA:HB1	1:130:A:MET:HE3	1	0.14
(1,552)	1:121:A:ALA:HB2	1:130:A:MET:HE1	1	0.14
(1,552)	1:121:A:ALA:HB2	1:130:A:MET:HE2	1	0.14
(1,552)	1:121:A:ALA:HB2	1:130:A:MET:HE3	1	0.14
(1,552)	1:121:A:ALA:HB3	1:130:A:MET:HE1	1	0.14
(1,552)	1:121:A:ALA:HB3	1:130:A:MET:HE2	1	0.14
(1,552)	1:121:A:ALA:HB3	1:130:A:MET:HE3	1	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	2	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	2	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	2	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	2	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	2	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	2	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	2	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	2	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	2	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	5	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	5	0.14
(1,550)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	5	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD11	5	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	5	0.14
(1,550)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	5	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD11	5	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD12	5	0.14
(1,550)	1:121:A:ALA:HB3	1:122:A:LEU:HD13	5	0.14
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG21	2	0.14
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG22	2	0.14
(1,545)	1:109:A:THR:HG21	1:136:A:VAL:HG23	2	0.14
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG21	2	0.14
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG22	2	0.14
(1,545)	1:109:A:THR:HG22	1:136:A:VAL:HG23	2	0.14
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG21	2	0.14
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG22	2	0.14
(1,545)	1:109:A:THR:HG23	1:136:A:VAL:HG23	2	0.14
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	3	0.14
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	3	0.14
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	3	0.14
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	3	0.14
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	3	0.14
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	3	0.14
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	3	0.14
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	3	0.14
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	5	0.14
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	5	0.14
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	5	0.14
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	5	0.14
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	5	0.14
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	5	0.14
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	5	0.14
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	5	0.14
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	5	0.14
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	1	0.14
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	1	0.14
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	1	0.14
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	1	0.14
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	1	0.14
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	1	0.14
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	1	0.14
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	1	0.14
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	1	0.14
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE1	10	0.14
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE2	10	0.14
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE3	10	0.14
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE1	10	0.14
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE2	10	0.14
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE3	10	0.14
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE1	10	0.14
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE2	10	0.14
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE3	10	0.14
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD11	10	0.14
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD12	10	0.14
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD13	10	0.14
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD11	10	0.14
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD12	10	0.14
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD13	10	0.14
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD11	10	0.14
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD12	10	0.14
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD13	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	7	0.14
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	7	0.14
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	7	0.14
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	7	0.14
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	7	0.14
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	7	0.14
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	7	0.14
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	7	0.14
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	7	0.14
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	2	0.14
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	2	0.14
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	2	0.14
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	2	0.14
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	2	0.14
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	2	0.14
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	2	0.14
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	2	0.14
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	2	0.14
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	9	0.14
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	9	0.14
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	9	0.14
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	9	0.14
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	9	0.14
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	9	0.14
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	9	0.14
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	9	0.14
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	9	0.14
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG21	6	0.14
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG22	6	0.14
(1,491)	1:80:A:LEU:HD11	1:207:A:VAL:HG23	6	0.14
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG21	6	0.14
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG22	6	0.14
(1,491)	1:80:A:LEU:HD12	1:207:A:VAL:HG23	6	0.14
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG21	6	0.14
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG22	6	0.14
(1,491)	1:80:A:LEU:HD13	1:207:A:VAL:HG23	6	0.14
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD11	10	0.14
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD12	10	0.14
(1,484)	1:59:A:ILE:HD11	1:96:A:ILE:HD13	10	0.14
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD11	10	0.14
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD12	10	0.14
(1,484)	1:59:A:ILE:HD12	1:96:A:ILE:HD13	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD11	10	0.14
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD12	10	0.14
(1,484)	1:59:A:ILE:HD13	1:96:A:ILE:HD13	10	0.14
(1,464)	1:48:A:LEU:HD11	1:186:A:VAL:HG21	3	0.14
(1,464)	1:48:A:LEU:HD11	1:186:A:VAL:HG22	3	0.14
(1,464)	1:48:A:LEU:HD11	1:186:A:VAL:HG23	3	0.14
(1,464)	1:48:A:LEU:HD12	1:186:A:VAL:HG21	3	0.14
(1,464)	1:48:A:LEU:HD12	1:186:A:VAL:HG22	3	0.14
(1,464)	1:48:A:LEU:HD12	1:186:A:VAL:HG23	3	0.14
(1,464)	1:48:A:LEU:HD13	1:186:A:VAL:HG21	3	0.14
(1,464)	1:48:A:LEU:HD13	1:186:A:VAL:HG22	3	0.14
(1,464)	1:48:A:LEU:HD13	1:186:A:VAL:HG23	3	0.14
(1,435)	1:32:A:LEU:HD21	1:128:A:ILE:HD11	8	0.14
(1,435)	1:32:A:LEU:HD21	1:128:A:ILE:HD12	8	0.14
(1,435)	1:32:A:LEU:HD21	1:128:A:ILE:HD13	8	0.14
(1,435)	1:32:A:LEU:HD22	1:128:A:ILE:HD11	8	0.14
(1,435)	1:32:A:LEU:HD22	1:128:A:ILE:HD12	8	0.14
(1,435)	1:32:A:LEU:HD22	1:128:A:ILE:HD13	8	0.14
(1,435)	1:32:A:LEU:HD23	1:128:A:ILE:HD11	8	0.14
(1,435)	1:32:A:LEU:HD23	1:128:A:ILE:HD12	8	0.14
(1,435)	1:32:A:LEU:HD23	1:128:A:ILE:HD13	8	0.14
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	3	0.14
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	3	0.14
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	3	0.14
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	3	0.14
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	3	0.14
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	3	0.14
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	3	0.14
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	3	0.14
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	3	0.14
(1,431)	1:32:A:LEU:HD21	1:115:A:THR:HG21	10	0.14
(1,431)	1:32:A:LEU:HD21	1:115:A:THR:HG22	10	0.14
(1,431)	1:32:A:LEU:HD21	1:115:A:THR:HG23	10	0.14
(1,431)	1:32:A:LEU:HD22	1:115:A:THR:HG21	10	0.14
(1,431)	1:32:A:LEU:HD22	1:115:A:THR:HG22	10	0.14
(1,431)	1:32:A:LEU:HD22	1:115:A:THR:HG23	10	0.14
(1,431)	1:32:A:LEU:HD23	1:115:A:THR:HG21	10	0.14
(1,431)	1:32:A:LEU:HD23	1:115:A:THR:HG22	10	0.14
(1,431)	1:32:A:LEU:HD23	1:115:A:THR:HG23	10	0.14
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	2	0.14
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	2	0.14
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	2	0.14
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	2	0.14
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	2	0.14
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	2	0.14
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	2	0.14
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	2	0.14
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG21	3	0.14
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG22	3	0.14
(1,408)	1:26:A:ILE:HD11	1:115:A:THR:HG23	3	0.14
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG21	3	0.14
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG22	3	0.14
(1,408)	1:26:A:ILE:HD12	1:115:A:THR:HG23	3	0.14
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG21	3	0.14
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG22	3	0.14
(1,408)	1:26:A:ILE:HD13	1:115:A:THR:HG23	3	0.14
(1,362)	1:159:A:GLN:H	1:175:A:ASP:H	6	0.14
(1,353)	1:149:A:THR:H	1:187:A:ILE:H	8	0.14
(1,351)	1:148:A:VAL:H	1:164:A:SER:H	8	0.14
(1,341)	1:95:A:GLY:H	1:184:A:THR:H	8	0.14
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	10	0.14
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	3	0.14
(1,299)	1:211:A:SER:H	1:214:A:ILE:H	5	0.14
(1,270)	1:104:A:ILE:H	1:107:A:LEU:H	6	0.14
(1,243)	1:224:A:LYS:H	1:226:A:ARG:H	5	0.14
(1,242)	1:223:A:GLU:H	1:225:A:GLU:H	9	0.14
(1,236)	1:210:A:HIS:H	1:212:A:GLN:H	5	0.14
(1,217)	1:180:A:MET:H	1:182:A:ARG:H	8	0.14
(1,192)	1:104:A:ILE:H	1:106:A:ASN:H	7	0.14
(1,184)	1:72:A:SER:H	1:74:A:LYS:H	1	0.14
(1,180)	1:68:A:SER:H	1:70:A:LEU:H	2	0.14
(1,121)	1:194:A:GLN:H	1:195:A:THR:H	4	0.14
(1,79)	1:137:A:GLY:H	1:138:A:PHE:H	5	0.14
(1,63)	1:105:A:ASN:H	1:106:A:ASN:H	3	0.14
(1,60)	1:102:A:ASP:H	1:103:A:LEU:H	4	0.14
(2,126)	1:59:A:ILE:H	1:55:A:ALA:O	10	0.13
(2,102)	1:47:A:GLU:H	1:43:A:ILE:O	9	0.13
(2,92)	1:33:A:ILE:H	1:29:A:LEU:O	6	0.13
(2,84)	1:29:A:LEU:H	1:25:A:GLU:O	3	0.13
(2,48)	1:148:A:VAL:H	1:164:A:SER:O	3	0.13
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	9	0.13
(2,30)	1:88:A:THR:H	1:83:A:ASN:O	6	0.13
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG12	10	0.13
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG13	10	0.13
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG11	5	0.13
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG12	5	0.13
(1,1112)	1:225:A:GLU:H	1:222:A:VAL:HG13	5	0.13
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG21	10	0.13
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG22	10	0.13
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG23	10	0.13
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	3	0.13
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	3	0.13
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	3	0.13
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	10	0.13
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	10	0.13
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	10	0.13
(1,1056)	1:200:A:GLU:H	1:203:A:ILE:HD11	8	0.13
(1,1056)	1:200:A:GLU:H	1:203:A:ILE:HD12	8	0.13
(1,1056)	1:200:A:GLU:H	1:203:A:ILE:HD13	8	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD11	3	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD12	3	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD13	3	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD11	7	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD12	7	0.13
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD13	7	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG21	5	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG22	5	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG23	5	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG21	6	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG22	6	0.13
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG23	6	0.13
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD21	8	0.13
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD22	8	0.13
(1,1014)	1:188:A:LEU:H	1:89:A:LEU:HD23	8	0.13
(1,987)	1:182:A:ARG:H	1:94:A:THR:HG21	2	0.13
(1,987)	1:182:A:ARG:H	1:94:A:THR:HG22	2	0.13
(1,987)	1:182:A:ARG:H	1:94:A:THR:HG23	2	0.13
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG21	1	0.13
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG22	1	0.13
(1,986)	1:177:A:GLY:H	1:176:A:THR:HG23	1	0.13
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG21	7	0.13
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG22	7	0.13
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG23	7	0.13
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG11	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG12	3	0.13
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG13	3	0.13
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG11	10	0.13
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG12	10	0.13
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG13	10	0.13
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	3	0.13
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	3	0.13
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	3	0.13
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG21	4	0.13
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG22	4	0.13
(1,965)	1:162:A:TRP:H	1:172:A:VAL:HG23	4	0.13
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	1	0.13
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	1	0.13
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	1	0.13
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG21	4	0.13
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG22	4	0.13
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG23	4	0.13
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG21	6	0.13
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG22	6	0.13
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG23	6	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG21	1	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG22	1	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG23	1	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG21	5	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG22	5	0.13
(1,928)	1:146:A:GLU:H	1:148:A:VAL:HG23	5	0.13
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG21	7	0.13
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG22	7	0.13
(1,904)	1:139:A:TYR:H	1:136:A:VAL:HG23	7	0.13
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	5	0.13
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	5	0.13
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	5	0.13
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	5	0.13
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	5	0.13
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	5	0.13
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	10	0.13
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	10	0.13
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	10	0.13
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD11	5	0.13
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD12	5	0.13
(1,858)	1:105:A:ASN:H	1:104:A:ILE:HD13	5	0.13
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD11	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD12	6	0.13
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD13	6	0.13
(1,844)	1:93:A:ASP:H	1:180:A:MET:HE1	9	0.13
(1,844)	1:93:A:ASP:H	1:180:A:MET:HE2	9	0.13
(1,844)	1:93:A:ASP:H	1:180:A:MET:HE3	9	0.13
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG21	4	0.13
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG22	4	0.13
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG23	4	0.13
(1,827)	1:89:A:LEU:H	1:190:A:LEU:HD21	7	0.13
(1,827)	1:89:A:LEU:H	1:190:A:LEU:HD22	7	0.13
(1,827)	1:89:A:LEU:H	1:190:A:LEU:HD23	7	0.13
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD21	9	0.13
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD22	9	0.13
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD23	9	0.13
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD11	4	0.13
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD12	4	0.13
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD13	4	0.13
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG21	4	0.13
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG22	4	0.13
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG23	4	0.13
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG21	1	0.13
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG22	1	0.13
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG23	1	0.13
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG21	5	0.13
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG22	5	0.13
(1,789)	1:78:A:ILE:H	1:94:A:THR:HG23	5	0.13
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD11	6	0.13
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD12	6	0.13
(1,765)	1:63:A:SER:H	1:59:A:ILE:HD13	6	0.13
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD21	5	0.13
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD22	5	0.13
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD23	5	0.13
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD11	1	0.13
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD12	1	0.13
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD13	1	0.13
(1,711)	1:33:A:ILE:H	1:131:A:ILE:HD11	2	0.13
(1,711)	1:33:A:ILE:H	1:131:A:ILE:HD12	2	0.13
(1,711)	1:33:A:ILE:H	1:131:A:ILE:HD13	2	0.13
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	1	0.13
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	1	0.13
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	1	0.13
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB1	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB2	4	0.13
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB3	4	0.13
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB1	5	0.13
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB2	5	0.13
(1,691)	1:22:A:PHE:H	1:21:A:ALA:HB3	5	0.13
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG11	10	0.13
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG12	10	0.13
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG13	10	0.13
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG21	4	0.13
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG22	4	0.13
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG23	4	0.13
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG11	8	0.13
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG12	8	0.13
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG13	8	0.13
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD11	8	0.13
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD12	8	0.13
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD13	8	0.13
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	5	0.13
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	5	0.13
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	5	0.13
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	5	0.13
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	5	0.13
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	5	0.13
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	5	0.13
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	5	0.13
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	5	0.13
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB1	7	0.13
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB2	7	0.13
(1,551)	1:121:A:ALA:HB1	1:126:A:ALA:HB3	7	0.13
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB1	7	0.13
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB2	7	0.13
(1,551)	1:121:A:ALA:HB2	1:126:A:ALA:HB3	7	0.13
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB1	7	0.13
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB2	7	0.13
(1,551)	1:121:A:ALA:HB3	1:126:A:ALA:HB3	7	0.13
(1,549)	1:119:A:MET:HE1	1:122:A:LEU:HD21	9	0.13
(1,549)	1:119:A:MET:HE1	1:122:A:LEU:HD22	9	0.13
(1,549)	1:119:A:MET:HE1	1:122:A:LEU:HD23	9	0.13
(1,549)	1:119:A:MET:HE2	1:122:A:LEU:HD21	9	0.13
(1,549)	1:119:A:MET:HE2	1:122:A:LEU:HD22	9	0.13
(1,549)	1:119:A:MET:HE2	1:122:A:LEU:HD23	9	0.13
(1,549)	1:119:A:MET:HE3	1:122:A:LEU:HD21	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:119:A:MET:HE3	1:122:A:LEU:HD22	9	0.13
(1,549)	1:119:A:MET:HE3	1:122:A:LEU:HD23	9	0.13
(1,542)	1:107:A:LEU:HD11	1:150:A:VAL:HG11	6	0.13
(1,542)	1:107:A:LEU:HD11	1:150:A:VAL:HG12	6	0.13
(1,542)	1:107:A:LEU:HD11	1:150:A:VAL:HG13	6	0.13
(1,542)	1:107:A:LEU:HD12	1:150:A:VAL:HG11	6	0.13
(1,542)	1:107:A:LEU:HD12	1:150:A:VAL:HG12	6	0.13
(1,542)	1:107:A:LEU:HD12	1:150:A:VAL:HG13	6	0.13
(1,542)	1:107:A:LEU:HD13	1:150:A:VAL:HG11	6	0.13
(1,542)	1:107:A:LEU:HD13	1:150:A:VAL:HG12	6	0.13
(1,542)	1:107:A:LEU:HD13	1:150:A:VAL:HG13	6	0.13
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	5	0.13
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	5	0.13
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	5	0.13
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	5	0.13
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	5	0.13
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	5	0.13
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	5	0.13
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	5	0.13
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	5	0.13
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG21	6	0.13
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG22	6	0.13
(1,532)	1:103:A:LEU:HD11	1:152:A:THR:HG23	6	0.13
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG21	6	0.13
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG22	6	0.13
(1,532)	1:103:A:LEU:HD12	1:152:A:THR:HG23	6	0.13
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG21	6	0.13
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG22	6	0.13
(1,532)	1:103:A:LEU:HD13	1:152:A:THR:HG23	6	0.13
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	3	0.13
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	3	0.13
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	3	0.13
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	3	0.13
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	3	0.13
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	3	0.13
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	3	0.13
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	3	0.13
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	3	0.13
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB1	7	0.13
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB2	7	0.13
(1,527)	1:99:A:THR:HG21	1:101:A:ALA:HB3	7	0.13
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB1	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB2	7	0.13
(1,527)	1:99:A:THR:HG22	1:101:A:ALA:HB3	7	0.13
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB1	7	0.13
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB2	7	0.13
(1,527)	1:99:A:THR:HG23	1:101:A:ALA:HB3	7	0.13
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD11	6	0.13
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD12	6	0.13
(1,521)	1:98:A:MET:HE1	1:107:A:LEU:HD13	6	0.13
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD11	6	0.13
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD12	6	0.13
(1,521)	1:98:A:MET:HE2	1:107:A:LEU:HD13	6	0.13
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD11	6	0.13
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD12	6	0.13
(1,521)	1:98:A:MET:HE3	1:107:A:LEU:HD13	6	0.13
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD11	4	0.13
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD12	4	0.13
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD13	4	0.13
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD11	4	0.13
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD12	4	0.13
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD13	4	0.13
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD11	4	0.13
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD12	4	0.13
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD13	4	0.13
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD11	10	0.13
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD12	10	0.13
(1,507)	1:89:A:LEU:HD21	1:203:A:ILE:HD13	10	0.13
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD11	10	0.13
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD12	10	0.13
(1,507)	1:89:A:LEU:HD22	1:203:A:ILE:HD13	10	0.13
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD11	10	0.13
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD12	10	0.13
(1,507)	1:89:A:LEU:HD23	1:203:A:ILE:HD13	10	0.13
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	1	0.13
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	1	0.13
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	1	0.13
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	1	0.13
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	1	0.13
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	1	0.13
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	1	0.13
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	1	0.13
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	1	0.13
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD12	10	0.13
(1,504)	1:89:A:LEU:HD21	1:188:A:LEU:HD13	10	0.13
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD11	10	0.13
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD12	10	0.13
(1,504)	1:89:A:LEU:HD22	1:188:A:LEU:HD13	10	0.13
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD11	10	0.13
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD12	10	0.13
(1,504)	1:89:A:LEU:HD23	1:188:A:LEU:HD13	10	0.13
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD11	3	0.13
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD12	3	0.13
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD13	3	0.13
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD11	3	0.13
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD12	3	0.13
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD13	3	0.13
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD11	3	0.13
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD12	3	0.13
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD13	3	0.13
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD11	4	0.13
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD12	4	0.13
(1,495)	1:80:A:LEU:HD21	1:91:A:ILE:HD13	4	0.13
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD11	4	0.13
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD12	4	0.13
(1,495)	1:80:A:LEU:HD22	1:91:A:ILE:HD13	4	0.13
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD11	4	0.13
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD12	4	0.13
(1,495)	1:80:A:LEU:HD23	1:91:A:ILE:HD13	4	0.13
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD11	5	0.13
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD12	5	0.13
(1,492)	1:80:A:LEU:HD11	1:218:A:ILE:HD13	5	0.13
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD11	5	0.13
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD12	5	0.13
(1,492)	1:80:A:LEU:HD12	1:218:A:ILE:HD13	5	0.13
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD11	5	0.13
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD12	5	0.13
(1,492)	1:80:A:LEU:HD13	1:218:A:ILE:HD13	5	0.13
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG11	10	0.13
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG12	10	0.13
(1,490)	1:80:A:LEU:HD11	1:207:A:VAL:HG13	10	0.13
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG11	10	0.13
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG12	10	0.13
(1,490)	1:80:A:LEU:HD12	1:207:A:VAL:HG13	10	0.13
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG11	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG12	10	0.13
(1,490)	1:80:A:LEU:HD13	1:207:A:VAL:HG13	10	0.13
(1,469)	1:48:A:LEU:HD21	1:188:A:LEU:HD11	10	0.13
(1,469)	1:48:A:LEU:HD21	1:188:A:LEU:HD12	10	0.13
(1,469)	1:48:A:LEU:HD21	1:188:A:LEU:HD13	10	0.13
(1,469)	1:48:A:LEU:HD22	1:188:A:LEU:HD11	10	0.13
(1,469)	1:48:A:LEU:HD22	1:188:A:LEU:HD12	10	0.13
(1,469)	1:48:A:LEU:HD22	1:188:A:LEU:HD13	10	0.13
(1,469)	1:48:A:LEU:HD23	1:188:A:LEU:HD11	10	0.13
(1,469)	1:48:A:LEU:HD23	1:188:A:LEU:HD12	10	0.13
(1,469)	1:48:A:LEU:HD23	1:188:A:LEU:HD13	10	0.13
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	3	0.13
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	3	0.13
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	3	0.13
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	3	0.13
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	3	0.13
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	3	0.13
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	3	0.13
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	3	0.13
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	3	0.13
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG21	1	0.13
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG22	1	0.13
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG23	1	0.13
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG21	1	0.13
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG22	1	0.13
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG23	1	0.13
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG21	1	0.13
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG22	1	0.13
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG23	1	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	3	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	3	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	3	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	3	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	3	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	3	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	3	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	3	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	3	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	8	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	8	0.13
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	8	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	8	0.13
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	8	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	8	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	8	0.13
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	8	0.13
(1,418)	1:29:A:LEU:HD11	1:136:A:VAL:HG11	4	0.13
(1,418)	1:29:A:LEU:HD11	1:136:A:VAL:HG12	4	0.13
(1,418)	1:29:A:LEU:HD11	1:136:A:VAL:HG13	4	0.13
(1,418)	1:29:A:LEU:HD12	1:136:A:VAL:HG11	4	0.13
(1,418)	1:29:A:LEU:HD12	1:136:A:VAL:HG12	4	0.13
(1,418)	1:29:A:LEU:HD12	1:136:A:VAL:HG13	4	0.13
(1,418)	1:29:A:LEU:HD13	1:136:A:VAL:HG11	4	0.13
(1,418)	1:29:A:LEU:HD13	1:136:A:VAL:HG12	4	0.13
(1,418)	1:29:A:LEU:HD13	1:136:A:VAL:HG13	4	0.13
(1,348)	1:146:A:GLU:H	1:191:A:LYS:H	4	0.13
(1,348)	1:146:A:GLU:H	1:191:A:LYS:H	7	0.13
(1,342)	1:103:A:LEU:H	1:107:A:LEU:H	5	0.13
(1,340)	1:93:A:ASP:H	1:186:A:VAL:H	8	0.13
(1,312)	1:56:A:LEU:H	1:96:A:ILE:H	5	0.13
(1,262)	1:69:A:LYS:H	1:72:A:SER:H	7	0.13
(1,247)	1:35:A:ASN:H	1:38:A:TYR:H	10	0.13
(1,242)	1:223:A:GLU:H	1:225:A:GLU:H	8	0.13
(1,217)	1:180:A:MET:H	1:182:A:ARG:H	1	0.13
(1,216)	1:167:A:GLY:H	1:169:A:SER:H	1	0.13
(1,73)	1:127:A:ASP:H	1:128:A:ILE:H	4	0.13
(1,63)	1:105:A:ASN:H	1:106:A:ASN:H	4	0.13
(1,11)	1:41:A:LYS:H	1:42:A:GLU:H	9	0.13
(1,10)	1:38:A:TYR:H	1:39:A:SER:H	2	0.13
(1,10)	1:38:A:TYR:H	1:39:A:SER:H	7	0.13
(2,144)	1:208:A:LYS:H	1:204:A:LYS:O	6	0.12
(2,92)	1:33:A:ILE:H	1:29:A:LEU:O	9	0.12
(2,80)	1:190:A:LEU:H	1:87:A:ARG:O	2	0.12
(2,80)	1:190:A:LEU:H	1:87:A:ARG:O	4	0.12
(2,68)	1:153:A:LYS:H	1:183:A:GLY:O	2	0.12
(2,44)	1:147:A:LYS:H	1:189:A:HIS:O	8	0.12
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG21	4	0.12
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG22	4	0.12
(1,1111)	1:223:A:GLU:H	1:222:A:VAL:HG23	4	0.12
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD11	10	0.12
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD12	10	0.12
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD13	10	0.12
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD11	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD12	6	0.12
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD13	6	0.12
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD11	10	0.12
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD12	10	0.12
(1,1095)	1:216:A:TYR:H	1:214:A:ILE:HD13	10	0.12
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG21	5	0.12
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG22	5	0.12
(1,1087)	1:210:A:HIS:H	1:207:A:VAL:HG23	5	0.12
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	4	0.12
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	4	0.12
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	4	0.12
(1,1071)	1:204:A:LYS:H	1:220:A:LEU:HD21	1	0.12
(1,1071)	1:204:A:LYS:H	1:220:A:LEU:HD22	1	0.12
(1,1071)	1:204:A:LYS:H	1:220:A:LEU:HD23	1	0.12
(1,1041)	1:196:A:GLU:H	1:190:A:LEU:HD21	4	0.12
(1,1041)	1:196:A:GLU:H	1:190:A:LEU:HD22	4	0.12
(1,1041)	1:196:A:GLU:H	1:190:A:LEU:HD23	4	0.12
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG21	5	0.12
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG22	5	0.12
(1,1036)	1:192:A:GLU:H	1:195:A:THR:HG23	5	0.12
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD21	2	0.12
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD22	2	0.12
(1,1035)	1:191:A:LYS:H	1:190:A:LEU:HD23	2	0.12
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG21	4	0.12
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG22	4	0.12
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG23	4	0.12
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG21	10	0.12
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG22	10	0.12
(1,1033)	1:191:A:LYS:H	1:144:A:VAL:HG23	10	0.12
(1,1015)	1:188:A:LEU:H	1:90:A:THR:HG21	4	0.12
(1,1015)	1:188:A:LEU:H	1:90:A:THR:HG22	4	0.12
(1,1015)	1:188:A:LEU:H	1:90:A:THR:HG23	4	0.12
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG21	10	0.12
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG22	10	0.12
(1,1013)	1:188:A:LEU:H	1:88:A:THR:HG23	10	0.12
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE1	7	0.12
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE2	7	0.12
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE3	7	0.12
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG21	6	0.12
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG22	6	0.12
(1,984)	1:175:A:ASP:H	1:174:A:THR:HG23	6	0.12
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB1	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB2	10	0.12
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB3	10	0.12
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD21	3	0.12
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD22	3	0.12
(1,979)	1:173:A:ARG:H	1:103:A:LEU:HD23	3	0.12
(1,974)	1:170:A:PHE:H	1:19:A:THR:HG21	1	0.12
(1,974)	1:170:A:PHE:H	1:19:A:THR:HG22	1	0.12
(1,974)	1:170:A:PHE:H	1:19:A:THR:HG23	1	0.12
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB1	6	0.12
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB2	6	0.12
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB3	6	0.12
(1,969)	1:163:A:GLU:H	1:172:A:VAL:HG11	10	0.12
(1,969)	1:163:A:GLU:H	1:172:A:VAL:HG12	10	0.12
(1,969)	1:163:A:GLU:H	1:172:A:VAL:HG13	10	0.12
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	7	0.12
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	7	0.12
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	7	0.12
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG21	8	0.12
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG22	8	0.12
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG23	8	0.12
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG21	5	0.12
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG22	5	0.12
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG23	5	0.12
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	1	0.12
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	1	0.12
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	1	0.12
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	7	0.12
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	7	0.12
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	7	0.12
(1,923)	1:145:A:ALA:H	1:148:A:VAL:HG21	8	0.12
(1,923)	1:145:A:ALA:H	1:148:A:VAL:HG22	8	0.12
(1,923)	1:145:A:ALA:H	1:148:A:VAL:HG23	8	0.12
(1,914)	1:142:A:TYR:H	1:148:A:VAL:HG11	4	0.12
(1,914)	1:142:A:TYR:H	1:148:A:VAL:HG12	4	0.12
(1,914)	1:142:A:TYR:H	1:148:A:VAL:HG13	4	0.12
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD11	8	0.12
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD12	8	0.12
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD13	8	0.12
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG11	3	0.12
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG12	3	0.12
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG13	3	0.12
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE1	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE2	7	0.12
(1,890)	1:131:A:ILE:H	1:130:A:MET:HE3	7	0.12
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD11	4	0.12
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD12	4	0.12
(1,887)	1:128:A:ILE:H	1:122:A:LEU:HD13	4	0.12
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD11	6	0.12
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD12	6	0.12
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD13	6	0.12
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	8	0.12
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	8	0.12
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	8	0.12
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG21	7	0.12
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG22	7	0.12
(1,842)	1:93:A:ASP:H	1:92:A:VAL:HG23	7	0.12
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	6	0.12
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	6	0.12
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	6	0.12
(1,793)	1:79:A:ASN:H	1:90:A:THR:HG21	2	0.12
(1,793)	1:79:A:ASN:H	1:90:A:THR:HG22	2	0.12
(1,793)	1:79:A:ASN:H	1:90:A:THR:HG23	2	0.12
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD21	5	0.12
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD22	5	0.12
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD23	5	0.12
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD21	10	0.12
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD22	10	0.12
(1,791)	1:79:A:ASN:H	1:80:A:LEU:HD23	10	0.12
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD21	5	0.12
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD22	5	0.12
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD23	5	0.12
(1,759)	1:61:A:TYR:H	1:64:A:LEU:HD11	6	0.12
(1,759)	1:61:A:TYR:H	1:64:A:LEU:HD12	6	0.12
(1,759)	1:61:A:TYR:H	1:64:A:LEU:HD13	6	0.12
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD11	3	0.12
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD12	3	0.12
(1,753)	1:60:A:ARG:H	1:59:A:ILE:HD13	3	0.12
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD21	7	0.12
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD22	7	0.12
(1,751)	1:59:A:ILE:H	1:76:A:LEU:HD23	7	0.12
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD21	7	0.12
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD22	7	0.12
(1,748)	1:57:A:ASP:H	1:56:A:LEU:HD23	7	0.12
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD12	4	0.12
(1,747)	1:57:A:ASP:H	1:56:A:LEU:HD13	4	0.12
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	5	0.12
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	5	0.12
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	5	0.12
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	8	0.12
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	8	0.12
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	8	0.12
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD21	10	0.12
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD22	10	0.12
(1,710)	1:33:A:ILE:H	1:32:A:LEU:HD23	10	0.12
(1,702)	1:31:A:SER:H	1:30:A:MET:HE1	7	0.12
(1,702)	1:31:A:SER:H	1:30:A:MET:HE2	7	0.12
(1,702)	1:31:A:SER:H	1:30:A:MET:HE3	7	0.12
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB1	1	0.12
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB2	1	0.12
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB3	1	0.12
(1,679)	1:222:A:VAL:H	1:222:A:VAL:HG21	9	0.12
(1,679)	1:222:A:VAL:H	1:222:A:VAL:HG22	9	0.12
(1,679)	1:222:A:VAL:H	1:222:A:VAL:HG23	9	0.12
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG21	1	0.12
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG22	1	0.12
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG23	1	0.12
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG21	2	0.12
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG22	2	0.12
(1,673)	1:207:A:VAL:H	1:207:A:VAL:HG23	2	0.12
(1,666)	1:190:A:LEU:H	1:190:A:LEU:HD11	1	0.12
(1,666)	1:190:A:LEU:H	1:190:A:LEU:HD12	1	0.12
(1,666)	1:190:A:LEU:H	1:190:A:LEU:HD13	1	0.12
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	1	0.12
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	1	0.12
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	1	0.12
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD21	8	0.12
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD22	8	0.12
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD23	8	0.12
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD11	2	0.12
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD12	2	0.12
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD13	2	0.12
(1,614)	1:33:A:ILE:H	1:33:A:ILE:HD11	2	0.12
(1,614)	1:33:A:ILE:H	1:33:A:ILE:HD12	2	0.12
(1,614)	1:33:A:ILE:H	1:33:A:ILE:HD13	2	0.12
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG21	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG22	9	0.12
(1,606)	1:220:A:LEU:HD21	1:222:A:VAL:HG23	9	0.12
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG21	9	0.12
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG22	9	0.12
(1,606)	1:220:A:LEU:HD22	1:222:A:VAL:HG23	9	0.12
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG21	9	0.12
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG22	9	0.12
(1,606)	1:220:A:LEU:HD23	1:222:A:VAL:HG23	9	0.12
(1,602)	1:214:A:ILE:HD11	1:218:A:ILE:HD11	1	0.12
(1,602)	1:214:A:ILE:HD11	1:218:A:ILE:HD12	1	0.12
(1,602)	1:214:A:ILE:HD11	1:218:A:ILE:HD13	1	0.12
(1,602)	1:214:A:ILE:HD12	1:218:A:ILE:HD11	1	0.12
(1,602)	1:214:A:ILE:HD12	1:218:A:ILE:HD12	1	0.12
(1,602)	1:214:A:ILE:HD12	1:218:A:ILE:HD13	1	0.12
(1,602)	1:214:A:ILE:HD13	1:218:A:ILE:HD11	1	0.12
(1,602)	1:214:A:ILE:HD13	1:218:A:ILE:HD12	1	0.12
(1,602)	1:214:A:ILE:HD13	1:218:A:ILE:HD13	1	0.12
(1,595)	1:190:A:LEU:HD21	1:198:A:LEU:HD21	3	0.12
(1,595)	1:190:A:LEU:HD21	1:198:A:LEU:HD22	3	0.12
(1,595)	1:190:A:LEU:HD21	1:198:A:LEU:HD23	3	0.12
(1,595)	1:190:A:LEU:HD22	1:198:A:LEU:HD21	3	0.12
(1,595)	1:190:A:LEU:HD22	1:198:A:LEU:HD22	3	0.12
(1,595)	1:190:A:LEU:HD22	1:198:A:LEU:HD23	3	0.12
(1,595)	1:190:A:LEU:HD23	1:198:A:LEU:HD21	3	0.12
(1,595)	1:190:A:LEU:HD23	1:198:A:LEU:HD22	3	0.12
(1,595)	1:190:A:LEU:HD23	1:198:A:LEU:HD23	3	0.12
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD11	6	0.12
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD12	6	0.12
(1,588)	1:186:A:VAL:HG11	1:188:A:LEU:HD13	6	0.12
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD11	6	0.12
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD12	6	0.12
(1,588)	1:186:A:VAL:HG12	1:188:A:LEU:HD13	6	0.12
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD11	6	0.12
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD12	6	0.12
(1,588)	1:186:A:VAL:HG13	1:188:A:LEU:HD13	6	0.12
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG11	4	0.12
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG12	4	0.12
(1,572)	1:148:A:VAL:HG11	1:150:A:VAL:HG13	4	0.12
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG11	4	0.12
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG12	4	0.12
(1,572)	1:148:A:VAL:HG12	1:150:A:VAL:HG13	4	0.12
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG12	4	0.12
(1,572)	1:148:A:VAL:HG13	1:150:A:VAL:HG13	4	0.12
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB1	7	0.12
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB2	7	0.12
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB3	7	0.12
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB1	7	0.12
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB2	7	0.12
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB3	7	0.12
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB1	7	0.12
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB2	7	0.12
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB3	7	0.12
(1,539)	1:103:A:LEU:HD21	1:172:A:VAL:HG21	2	0.12
(1,539)	1:103:A:LEU:HD21	1:172:A:VAL:HG22	2	0.12
(1,539)	1:103:A:LEU:HD21	1:172:A:VAL:HG23	2	0.12
(1,539)	1:103:A:LEU:HD22	1:172:A:VAL:HG21	2	0.12
(1,539)	1:103:A:LEU:HD22	1:172:A:VAL:HG22	2	0.12
(1,539)	1:103:A:LEU:HD22	1:172:A:VAL:HG23	2	0.12
(1,539)	1:103:A:LEU:HD23	1:172:A:VAL:HG21	2	0.12
(1,539)	1:103:A:LEU:HD23	1:172:A:VAL:HG22	2	0.12
(1,539)	1:103:A:LEU:HD23	1:172:A:VAL:HG23	2	0.12
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG21	6	0.12
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG22	6	0.12
(1,531)	1:103:A:LEU:HD11	1:150:A:VAL:HG23	6	0.12
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG21	6	0.12
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG22	6	0.12
(1,531)	1:103:A:LEU:HD12	1:150:A:VAL:HG23	6	0.12
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG21	6	0.12
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG22	6	0.12
(1,531)	1:103:A:LEU:HD13	1:150:A:VAL:HG23	6	0.12
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD21	1	0.12
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD22	1	0.12
(1,529)	1:103:A:LEU:HD11	1:107:A:LEU:HD23	1	0.12
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD21	1	0.12
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD22	1	0.12
(1,529)	1:103:A:LEU:HD12	1:107:A:LEU:HD23	1	0.12
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD21	1	0.12
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD22	1	0.12
(1,529)	1:103:A:LEU:HD13	1:107:A:LEU:HD23	1	0.12
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG21	4	0.12
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG22	4	0.12
(1,524)	1:98:A:MET:HE1	1:150:A:VAL:HG23	4	0.12
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG21	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG22	4	0.12
(1,524)	1:98:A:MET:HE2	1:150:A:VAL:HG23	4	0.12
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG21	4	0.12
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG22	4	0.12
(1,524)	1:98:A:MET:HE3	1:150:A:VAL:HG23	4	0.12
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE1	6	0.12
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE2	6	0.12
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE3	6	0.12
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE1	6	0.12
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE2	6	0.12
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE3	6	0.12
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE1	6	0.12
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE2	6	0.12
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE3	6	0.12
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG21	5	0.12
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG22	5	0.12
(1,512)	1:91:A:ILE:HD11	1:186:A:VAL:HG23	5	0.12
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG21	5	0.12
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG22	5	0.12
(1,512)	1:91:A:ILE:HD12	1:186:A:VAL:HG23	5	0.12
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG21	5	0.12
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG22	5	0.12
(1,512)	1:91:A:ILE:HD13	1:186:A:VAL:HG23	5	0.12
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	2	0.12
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	2	0.12
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	2	0.12
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	2	0.12
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	2	0.12
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	2	0.12
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	2	0.12
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	2	0.12
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	2	0.12
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	2	0.12
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	2	0.12
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	2	0.12
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	2	0.12
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	2	0.12
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	2	0.12
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	2	0.12
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	2	0.12
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	2	0.12
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	3	0.12
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	3	0.12
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	3	0.12
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	3	0.12
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	3	0.12
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	3	0.12
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	3	0.12
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	3	0.12
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD11	10	0.12
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD12	10	0.12
(1,487)	1:70:A:LEU:HD21	1:76:A:LEU:HD13	10	0.12
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD11	10	0.12
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD12	10	0.12
(1,487)	1:70:A:LEU:HD22	1:76:A:LEU:HD13	10	0.12
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD11	10	0.12
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD12	10	0.12
(1,487)	1:70:A:LEU:HD23	1:76:A:LEU:HD13	10	0.12
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	9	0.12
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	9	0.12
(1,486)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	9	0.12
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	9	0.12
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	9	0.12
(1,486)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	9	0.12
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	9	0.12
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	9	0.12
(1,486)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	9	0.12
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	1	0.12
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	1	0.12
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	1	0.12
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	1	0.12
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	1	0.12
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	1	0.12
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	1	0.12
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	1	0.12
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	1	0.12
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG11	1	0.12
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG12	1	0.12
(1,467)	1:48:A:LEU:HD21	1:186:A:VAL:HG13	1	0.12
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG11	1	0.12
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG12	1	0.12
(1,467)	1:48:A:LEU:HD22	1:186:A:VAL:HG13	1	0.12
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG11	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG12	1	0.12
(1,467)	1:48:A:LEU:HD23	1:186:A:VAL:HG13	1	0.12
(1,460)	1:45:A:LEU:HD21	1:206:A:ILE:HD11	10	0.12
(1,460)	1:45:A:LEU:HD21	1:206:A:ILE:HD12	10	0.12
(1,460)	1:45:A:LEU:HD21	1:206:A:ILE:HD13	10	0.12
(1,460)	1:45:A:LEU:HD22	1:206:A:ILE:HD11	10	0.12
(1,460)	1:45:A:LEU:HD22	1:206:A:ILE:HD12	10	0.12
(1,460)	1:45:A:LEU:HD22	1:206:A:ILE:HD13	10	0.12
(1,460)	1:45:A:LEU:HD23	1:206:A:ILE:HD11	10	0.12
(1,460)	1:45:A:LEU:HD23	1:206:A:ILE:HD12	10	0.12
(1,460)	1:45:A:LEU:HD23	1:206:A:ILE:HD13	10	0.12
(1,450)	1:45:A:LEU:HD11	1:206:A:ILE:HD11	9	0.12
(1,450)	1:45:A:LEU:HD11	1:206:A:ILE:HD12	9	0.12
(1,450)	1:45:A:LEU:HD11	1:206:A:ILE:HD13	9	0.12
(1,450)	1:45:A:LEU:HD12	1:206:A:ILE:HD11	9	0.12
(1,450)	1:45:A:LEU:HD12	1:206:A:ILE:HD12	9	0.12
(1,450)	1:45:A:LEU:HD12	1:206:A:ILE:HD13	9	0.12
(1,450)	1:45:A:LEU:HD13	1:206:A:ILE:HD11	9	0.12
(1,450)	1:45:A:LEU:HD13	1:206:A:ILE:HD12	9	0.12
(1,450)	1:45:A:LEU:HD13	1:206:A:ILE:HD13	9	0.12
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	4	0.12
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	4	0.12
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	4	0.12
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	4	0.12
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	4	0.12
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	4	0.12
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	4	0.12
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	4	0.12
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	4	0.12
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD11	9	0.12
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD12	9	0.12
(1,433)	1:32:A:LEU:HD21	1:122:A:LEU:HD13	9	0.12
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD11	9	0.12
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD12	9	0.12
(1,433)	1:32:A:LEU:HD22	1:122:A:LEU:HD13	9	0.12
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD11	9	0.12
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD12	9	0.12
(1,433)	1:32:A:LEU:HD23	1:122:A:LEU:HD13	9	0.12
(1,432)	1:32:A:LEU:HD21	1:119:A:MET:HE1	2	0.12
(1,432)	1:32:A:LEU:HD21	1:119:A:MET:HE2	2	0.12
(1,432)	1:32:A:LEU:HD21	1:119:A:MET:HE3	2	0.12
(1,432)	1:32:A:LEU:HD22	1:119:A:MET:HE1	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:32:A:LEU:HD22	1:119:A:MET:HE2	2	0.12
(1,432)	1:32:A:LEU:HD22	1:119:A:MET:HE3	2	0.12
(1,432)	1:32:A:LEU:HD23	1:119:A:MET:HE1	2	0.12
(1,432)	1:32:A:LEU:HD23	1:119:A:MET:HE2	2	0.12
(1,432)	1:32:A:LEU:HD23	1:119:A:MET:HE3	2	0.12
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD11	6	0.12
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD12	6	0.12
(1,429)	1:32:A:LEU:HD11	1:122:A:LEU:HD13	6	0.12
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD11	6	0.12
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD12	6	0.12
(1,429)	1:32:A:LEU:HD12	1:122:A:LEU:HD13	6	0.12
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD11	6	0.12
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD12	6	0.12
(1,429)	1:32:A:LEU:HD13	1:122:A:LEU:HD13	6	0.12
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB1	9	0.12
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB2	9	0.12
(1,427)	1:30:A:MET:HE1	1:166:A:ALA:HB3	9	0.12
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB1	9	0.12
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB2	9	0.12
(1,427)	1:30:A:MET:HE2	1:166:A:ALA:HB3	9	0.12
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB1	9	0.12
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB2	9	0.12
(1,427)	1:30:A:MET:HE3	1:166:A:ALA:HB3	9	0.12
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD11	5	0.12
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD12	5	0.12
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD13	5	0.12
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD11	5	0.12
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD12	5	0.12
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD13	5	0.12
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD11	5	0.12
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD12	5	0.12
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD13	5	0.12
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG21	7	0.12
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG22	7	0.12
(1,421)	1:29:A:LEU:HD21	1:115:A:THR:HG23	7	0.12
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG21	7	0.12
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG22	7	0.12
(1,421)	1:29:A:LEU:HD22	1:115:A:THR:HG23	7	0.12
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG21	7	0.12
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG22	7	0.12
(1,421)	1:29:A:LEU:HD23	1:115:A:THR:HG23	7	0.12
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	4	0.12
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	4	0.12
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	4	0.12
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	4	0.12
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	4	0.12
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	4	0.12
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	4	0.12
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	4	0.12
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD21	1	0.12
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD22	1	0.12
(1,406)	1:26:A:ILE:HD11	1:29:A:LEU:HD23	1	0.12
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD21	1	0.12
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD22	1	0.12
(1,406)	1:26:A:ILE:HD12	1:29:A:LEU:HD23	1	0.12
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD21	1	0.12
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD22	1	0.12
(1,406)	1:26:A:ILE:HD13	1:29:A:LEU:HD23	1	0.12
(1,374)	1:225:A:GLU:H	1:230:A:VAL:H	7	0.12
(1,355)	1:150:A:VAL:H	1:162:A:TRP:H	1	0.12
(1,353)	1:149:A:THR:H	1:187:A:ILE:H	7	0.12
(1,353)	1:149:A:THR:H	1:187:A:ILE:H	9	0.12
(1,344)	1:117:A:ALA:H	1:121:A:ALA:H	9	0.12
(1,342)	1:103:A:LEU:H	1:107:A:LEU:H	9	0.12
(1,312)	1:56:A:LEU:H	1:96:A:ILE:H	9	0.12
(1,281)	1:136:A:VAL:H	1:139:A:TYR:H	8	0.12
(1,278)	1:131:A:ILE:H	1:134:A:PHE:H	9	0.12
(1,268)	1:101:A:ALA:H	1:104:A:ILE:H	4	0.12
(1,262)	1:69:A:LYS:H	1:72:A:SER:H	3	0.12
(1,261)	1:68:A:SER:H	1:71:A:ASP:H	1	0.12
(1,237)	1:211:A:SER:H	1:213:A:PHE:H	6	0.12
(1,222)	1:194:A:GLN:H	1:196:A:GLU:H	6	0.12
(1,210)	1:139:A:TYR:H	1:141:A:ALA:H	5	0.12
(1,200)	1:123:A:GLN:H	1:125:A:GLY:H	8	0.12
(1,182)	1:70:A:LEU:H	1:72:A:SER:H	1	0.12
(1,178)	1:64:A:LEU:H	1:66:A:ASP:H	6	0.12
(1,142)	1:215:A:GLY:H	1:216:A:TYR:H	7	0.12
(1,101)	1:168:A:GLY:H	1:169:A:SER:H	4	0.12
(1,80)	1:138:A:PHE:H	1:139:A:TYR:H	8	0.12
(1,74)	1:128:A:ILE:H	1:129:A:SER:H	9	0.12
(1,41)	1:76:A:LEU:H	1:77:A:HIS:H	10	0.12
(1,39)	1:74:A:LYS:H	1:75:A:GLU:H	1	0.12
(2,150)	1:211:A:SER:H	1:207:A:VAL:O	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:55:A:ALA:H	1:51:A:ASN:O	2	0.11
(2,97)	1:44:A:PHE:N	1:41:A:LYS:O	4	0.11
(2,96)	1:35:A:ASN:H	1:31:A:SER:O	7	0.11
(2,66)	1:160:A:TYR:H	1:152:A:THR:O	6	0.11
(2,64)	1:152:A:THR:H	1:160:A:TYR:O	4	0.11
(2,47)	1:148:A:VAL:N	1:164:A:SER:O	3	0.11
(2,40)	1:93:A:ASP:H	1:184:A:THR:O	8	0.11
(2,12)	1:78:A:ILE:H	1:217:A:PRO:O	6	0.11
(2,10)	1:22:A:PHE:H	1:168:A:GLY:O	4	0.11
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD11	8	0.11
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD12	8	0.11
(1,1096)	1:216:A:TYR:H	1:218:A:ILE:HD13	8	0.11
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG21	4	0.11
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG22	4	0.11
(1,1085)	1:209:A:LYS:H	1:207:A:VAL:HG23	4	0.11
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD11	5	0.11
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD12	5	0.11
(1,1080)	1:207:A:VAL:H	1:206:A:ILE:HD13	5	0.11
(1,1073)	1:205:A:GLU:H	1:207:A:VAL:HG11	7	0.11
(1,1073)	1:205:A:GLU:H	1:207:A:VAL:HG12	7	0.11
(1,1073)	1:205:A:GLU:H	1:207:A:VAL:HG13	7	0.11
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG21	7	0.11
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG22	7	0.11
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG23	7	0.11
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG21	8	0.11
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG22	8	0.11
(1,1050)	1:198:A:LEU:H	1:195:A:THR:HG23	8	0.11
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD11	9	0.11
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD12	9	0.11
(1,1047)	1:197:A:TYR:H	1:198:A:LEU:HD13	9	0.11
(1,1039)	1:194:A:GLN:H	1:195:A:THR:HG21	1	0.11
(1,1039)	1:194:A:GLN:H	1:195:A:THR:HG22	1	0.11
(1,1039)	1:194:A:GLN:H	1:195:A:THR:HG23	1	0.11
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD21	4	0.11
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD22	4	0.11
(1,1011)	1:187:A:ILE:H	1:188:A:LEU:HD23	4	0.11
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE1	9	0.11
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE2	9	0.11
(1,995)	1:185:A:LYS:H	1:180:A:MET:HE3	9	0.11
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB1	5	0.11
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB2	5	0.11
(1,983)	1:175:A:ASP:H	1:161:A:ALA:HB3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:173:A:ARG:H	1:161:A:ALA:HB1	4	0.11
(1,980)	1:173:A:ARG:H	1:161:A:ALA:HB2	4	0.11
(1,980)	1:173:A:ARG:H	1:161:A:ALA:HB3	4	0.11
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB1	10	0.11
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB2	10	0.11
(1,973)	1:169:A:SER:H	1:166:A:ALA:HB3	10	0.11
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG11	7	0.11
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG12	7	0.11
(1,970)	1:164:A:SER:H	1:148:A:VAL:HG13	7	0.11
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG21	7	0.11
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG22	7	0.11
(1,966)	1:163:A:GLU:H	1:149:A:THR:HG23	7	0.11
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB1	3	0.11
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB2	3	0.11
(1,963)	1:162:A:TRP:H	1:161:A:ALA:HB3	3	0.11
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG21	4	0.11
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG22	4	0.11
(1,953)	1:160:A:TYR:H	1:152:A:THR:HG23	4	0.11
(1,951)	1:159:A:GLN:H	1:174:A:THR:HG21	5	0.11
(1,951)	1:159:A:GLN:H	1:174:A:THR:HG22	5	0.11
(1,951)	1:159:A:GLN:H	1:174:A:THR:HG23	5	0.11
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG21	10	0.11
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG22	10	0.11
(1,949)	1:153:A:LYS:H	1:152:A:THR:HG23	10	0.11
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG21	9	0.11
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG22	9	0.11
(1,941)	1:151:A:ILE:H	1:149:A:THR:HG23	9	0.11
(1,939)	1:151:A:ILE:H	1:98:A:MET:HE1	8	0.11
(1,939)	1:151:A:ILE:H	1:98:A:MET:HE2	8	0.11
(1,939)	1:151:A:ILE:H	1:98:A:MET:HE3	8	0.11
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD21	2	0.11
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD22	2	0.11
(1,929)	1:146:A:GLU:H	1:190:A:LEU:HD23	2	0.11
(1,926)	1:145:A:ALA:H	1:190:A:LEU:HD21	3	0.11
(1,926)	1:145:A:ALA:H	1:190:A:LEU:HD22	3	0.11
(1,926)	1:145:A:ALA:H	1:190:A:LEU:HD23	3	0.11
(1,919)	1:144:A:VAL:H	1:188:A:LEU:HD21	3	0.11
(1,919)	1:144:A:VAL:H	1:188:A:LEU:HD22	3	0.11
(1,919)	1:144:A:VAL:H	1:188:A:LEU:HD23	3	0.11
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG21	2	0.11
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG22	2	0.11
(1,918)	1:144:A:VAL:H	1:148:A:VAL:HG23	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG21	10	0.11
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG22	10	0.11
(1,917)	1:143:A:LEU:H	1:144:A:VAL:HG23	10	0.11
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD11	8	0.11
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD12	8	0.11
(1,911)	1:142:A:TYR:H	1:143:A:LEU:HD13	8	0.11
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD21	8	0.11
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD22	8	0.11
(1,900)	1:139:A:TYR:H	1:29:A:LEU:HD23	8	0.11
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD11	6	0.11
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD12	6	0.11
(1,896)	1:138:A:PHE:H	1:48:A:LEU:HD13	6	0.11
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG11	8	0.11
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG12	8	0.11
(1,894)	1:137:A:GLY:H	1:136:A:VAL:HG13	8	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG11	9	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG12	9	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG13	9	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG11	10	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG12	10	0.11
(1,891)	1:133:A:GLN:H	1:136:A:VAL:HG13	10	0.11
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD11	2	0.11
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD12	2	0.11
(1,884)	1:127:A:ASP:H	1:122:A:LEU:HD13	2	0.11
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE1	8	0.11
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE2	8	0.11
(1,882)	1:126:A:ALA:H	1:130:A:MET:HE3	8	0.11
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB1	2	0.11
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB2	2	0.11
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB3	2	0.11
(1,876)	1:123:A:GLN:H	1:126:A:ALA:HB1	7	0.11
(1,876)	1:123:A:GLN:H	1:126:A:ALA:HB2	7	0.11
(1,876)	1:123:A:GLN:H	1:126:A:ALA:HB3	7	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB1	7	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB2	7	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB3	7	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB1	8	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB2	8	0.11
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB3	8	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD21	1	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD22	1	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD23	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD21	6	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD22	6	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD23	6	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD21	9	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD22	9	0.11
(1,855)	1:104:A:ILE:H	1:103:A:LEU:HD23	9	0.11
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	3	0.11
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	3	0.11
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	3	0.11
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	6	0.11
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	6	0.11
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	6	0.11
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG21	9	0.11
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG22	9	0.11
(1,845)	1:93:A:ASP:H	1:184:A:THR:HG23	9	0.11
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG21	2	0.11
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG22	2	0.11
(1,839)	1:92:A:VAL:H	1:90:A:THR:HG23	2	0.11
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD21	1	0.11
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD22	1	0.11
(1,837)	1:92:A:VAL:H	1:80:A:LEU:HD23	1	0.11
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG21	2	0.11
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG22	2	0.11
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG23	2	0.11
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD21	2	0.11
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD22	2	0.11
(1,812)	1:83:A:ASN:H	1:198:A:LEU:HD23	2	0.11
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	2	0.11
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	2	0.11
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	2	0.11
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	3	0.11
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	3	0.11
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	3	0.11
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD11	3	0.11
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD12	3	0.11
(1,807)	1:81:A:ILE:H	1:220:A:LEU:HD13	3	0.11
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG21	6	0.11
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG22	6	0.11
(1,803)	1:81:A:ILE:H	1:90:A:THR:HG23	6	0.11
(1,788)	1:78:A:ILE:H	1:56:A:LEU:HD21	1	0.11
(1,788)	1:78:A:ILE:H	1:56:A:LEU:HD22	1	0.11
(1,788)	1:78:A:ILE:H	1:56:A:LEU:HD23	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD11	10	0.11
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD12	10	0.11
(1,787)	1:78:A:ILE:H	1:56:A:LEU:HD13	10	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD11	4	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD12	4	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD13	4	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD11	9	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD12	9	0.11
(1,782)	1:75:A:GLU:H	1:76:A:LEU:HD13	9	0.11
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD21	7	0.11
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD22	7	0.11
(1,754)	1:60:A:ARG:H	1:70:A:LEU:HD23	7	0.11
(1,707)	1:32:A:LEU:H	1:34:A:ILE:HD11	5	0.11
(1,707)	1:32:A:LEU:H	1:34:A:ILE:HD12	5	0.11
(1,707)	1:32:A:LEU:H	1:34:A:ILE:HD13	5	0.11
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB1	7	0.11
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB2	7	0.11
(1,704)	1:31:A:SER:H	1:166:A:ALA:HB3	7	0.11
(1,702)	1:31:A:SER:H	1:30:A:MET:HE1	1	0.11
(1,702)	1:31:A:SER:H	1:30:A:MET:HE2	1	0.11
(1,702)	1:31:A:SER:H	1:30:A:MET:HE3	1	0.11
(1,701)	1:29:A:LEU:H	1:119:A:MET:HE1	2	0.11
(1,701)	1:29:A:LEU:H	1:119:A:MET:HE2	2	0.11
(1,701)	1:29:A:LEU:H	1:119:A:MET:HE3	2	0.11
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	4	0.11
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	4	0.11
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	4	0.11
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB1	6	0.11
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB2	6	0.11
(1,698)	1:28:A:GLN:H	1:27:A:ALA:HB3	6	0.11
(1,696)	1:27:A:ALA:H	1:111:A:ALA:HB1	9	0.11
(1,696)	1:27:A:ALA:H	1:111:A:ALA:HB2	9	0.11
(1,696)	1:27:A:ALA:H	1:111:A:ALA:HB3	9	0.11
(1,689)	1:21:A:ALA:H	1:19:A:THR:HG21	10	0.11
(1,689)	1:21:A:ALA:H	1:19:A:THR:HG22	10	0.11
(1,689)	1:21:A:ALA:H	1:19:A:THR:HG23	10	0.11
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	8	0.11
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	8	0.11
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	8	0.11
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD21	7	0.11
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD22	7	0.11
(1,643)	1:107:A:LEU:H	1:107:A:LEU:HD23	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD11	4	0.11
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD12	4	0.11
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD13	4	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG21	3	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG22	3	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG23	3	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG21	3	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG22	3	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG23	3	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG21	3	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG22	3	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG23	3	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG21	4	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG22	4	0.11
(1,592)	1:190:A:LEU:HD11	1:195:A:THR:HG23	4	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG21	4	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG22	4	0.11
(1,592)	1:190:A:LEU:HD12	1:195:A:THR:HG23	4	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG21	4	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG22	4	0.11
(1,592)	1:190:A:LEU:HD13	1:195:A:THR:HG23	4	0.11
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG21	5	0.11
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG22	5	0.11
(1,580)	1:150:A:VAL:HG21	1:184:A:THR:HG23	5	0.11
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG21	5	0.11
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG22	5	0.11
(1,580)	1:150:A:VAL:HG22	1:184:A:THR:HG23	5	0.11
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG21	5	0.11
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG22	5	0.11
(1,580)	1:150:A:VAL:HG23	1:184:A:THR:HG23	5	0.11
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG21	1	0.11
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG22	1	0.11
(1,579)	1:150:A:VAL:HG21	1:152:A:THR:HG23	1	0.11
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG21	1	0.11
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG22	1	0.11
(1,579)	1:150:A:VAL:HG22	1:152:A:THR:HG23	1	0.11
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG21	1	0.11
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG22	1	0.11
(1,579)	1:150:A:VAL:HG23	1:152:A:THR:HG23	1	0.11
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB1	2	0.11
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB2	2	0.11
(1,575)	1:149:A:THR:HG21	1:161:A:ALA:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB1	2	0.11
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB2	2	0.11
(1,575)	1:149:A:THR:HG22	1:161:A:ALA:HB3	2	0.11
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB1	2	0.11
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB2	2	0.11
(1,575)	1:149:A:THR:HG23	1:161:A:ALA:HB3	2	0.11
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB1	4	0.11
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB2	4	0.11
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB3	4	0.11
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB1	4	0.11
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB2	4	0.11
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB3	4	0.11
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB1	4	0.11
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB2	4	0.11
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB3	4	0.11
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG21	6	0.11
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG22	6	0.11
(1,536)	1:103:A:LEU:HD21	1:150:A:VAL:HG23	6	0.11
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG21	6	0.11
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG22	6	0.11
(1,536)	1:103:A:LEU:HD22	1:150:A:VAL:HG23	6	0.11
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG21	6	0.11
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG22	6	0.11
(1,536)	1:103:A:LEU:HD23	1:150:A:VAL:HG23	6	0.11
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG11	10	0.11
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG12	10	0.11
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG13	10	0.11
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG11	10	0.11
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG12	10	0.11
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG13	10	0.11
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG11	10	0.11
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG12	10	0.11
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG13	10	0.11
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG11	9	0.11
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG12	9	0.11
(1,523)	1:98:A:MET:HE1	1:150:A:VAL:HG13	9	0.11
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG11	9	0.11
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG12	9	0.11
(1,523)	1:98:A:MET:HE2	1:150:A:VAL:HG13	9	0.11
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG11	9	0.11
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG12	9	0.11
(1,523)	1:98:A:MET:HE3	1:150:A:VAL:HG13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE1	4	0.11
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE2	4	0.11
(1,517)	1:92:A:VAL:HG21	1:180:A:MET:HE3	4	0.11
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE1	4	0.11
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE2	4	0.11
(1,517)	1:92:A:VAL:HG22	1:180:A:MET:HE3	4	0.11
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE1	4	0.11
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE2	4	0.11
(1,517)	1:92:A:VAL:HG23	1:180:A:MET:HE3	4	0.11
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD21	3	0.11
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD22	3	0.11
(1,505)	1:89:A:LEU:HD21	1:190:A:LEU:HD23	3	0.11
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD21	3	0.11
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD22	3	0.11
(1,505)	1:89:A:LEU:HD22	1:190:A:LEU:HD23	3	0.11
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD21	3	0.11
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD22	3	0.11
(1,505)	1:89:A:LEU:HD23	1:190:A:LEU:HD23	3	0.11
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD11	3	0.11
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD12	3	0.11
(1,503)	1:89:A:LEU:HD21	1:91:A:ILE:HD13	3	0.11
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD11	3	0.11
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD12	3	0.11
(1,503)	1:89:A:LEU:HD22	1:91:A:ILE:HD13	3	0.11
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD11	3	0.11
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD12	3	0.11
(1,503)	1:89:A:LEU:HD23	1:91:A:ILE:HD13	3	0.11
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD11	4	0.11
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD12	4	0.11
(1,500)	1:89:A:LEU:HD11	1:91:A:ILE:HD13	4	0.11
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD11	4	0.11
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD12	4	0.11
(1,500)	1:89:A:LEU:HD12	1:91:A:ILE:HD13	4	0.11
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD11	4	0.11
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD12	4	0.11
(1,500)	1:89:A:LEU:HD13	1:91:A:ILE:HD13	4	0.11
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD11	1	0.11
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD12	1	0.11
(1,494)	1:80:A:LEU:HD21	1:89:A:LEU:HD13	1	0.11
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD11	1	0.11
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD12	1	0.11
(1,494)	1:80:A:LEU:HD22	1:89:A:LEU:HD13	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD11	1	0.11
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD12	1	0.11
(1,494)	1:80:A:LEU:HD23	1:89:A:LEU:HD13	1	0.11
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	6	0.11
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	6	0.11
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	6	0.11
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	6	0.11
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	6	0.11
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	6	0.11
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	6	0.11
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	6	0.11
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	6	0.11
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	7	0.11
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	7	0.11
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	7	0.11
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	7	0.11
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	7	0.11
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	7	0.11
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	7	0.11
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	7	0.11
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	7	0.11
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD11	5	0.11
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD12	5	0.11
(1,475)	1:49:A:ILE:HD11	1:214:A:ILE:HD13	5	0.11
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD11	5	0.11
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD12	5	0.11
(1,475)	1:49:A:ILE:HD12	1:214:A:ILE:HD13	5	0.11
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD11	5	0.11
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD12	5	0.11
(1,475)	1:49:A:ILE:HD13	1:214:A:ILE:HD13	5	0.11
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD11	7	0.11
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD12	7	0.11
(1,423)	1:29:A:LEU:HD21	1:131:A:ILE:HD13	7	0.11
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD11	7	0.11
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD12	7	0.11
(1,423)	1:29:A:LEU:HD22	1:131:A:ILE:HD13	7	0.11
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD11	7	0.11
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD12	7	0.11
(1,423)	1:29:A:LEU:HD23	1:131:A:ILE:HD13	7	0.11
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD11	5	0.11
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD12	5	0.11
(1,420)	1:29:A:LEU:HD21	1:33:A:ILE:HD13	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD11	5	0.11
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD12	5	0.11
(1,420)	1:29:A:LEU:HD22	1:33:A:ILE:HD13	5	0.11
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD11	5	0.11
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD12	5	0.11
(1,420)	1:29:A:LEU:HD23	1:33:A:ILE:HD13	5	0.11
(1,372)	1:206:A:ILE:H	1:210:A:HIS:H	7	0.11
(1,368)	1:198:A:LEU:H	1:203:A:ILE:H	10	0.11
(1,337)	1:89:A:LEU:H	1:190:A:LEU:H	8	0.11
(1,318)	1:77:A:HIS:H	1:95:A:GLY:H	3	0.11
(1,306)	1:22:A:PHE:H	1:170:A:PHE:H	3	0.11
(1,281)	1:136:A:VAL:H	1:139:A:TYR:H	6	0.11
(1,243)	1:224:A:LYS:H	1:226:A:ARG:H	6	0.11
(1,243)	1:224:A:LYS:H	1:226:A:ARG:H	10	0.11
(1,217)	1:180:A:MET:H	1:182:A:ARG:H	3	0.11
(1,183)	1:71:A:ASP:H	1:73:A:GLY:H	7	0.11
(1,153)	1:24:A:ALA:H	1:26:A:ILE:H	7	0.11
(1,35)	1:69:A:LYS:H	1:70:A:LEU:H	9	0.11
(1,33)	1:65:A:THR:H	1:66:A:ASP:H	3	0.11
(1,10)	1:38:A:TYR:H	1:39:A:SER:H	10	0.11
(2,106)	1:49:A:ILE:H	1:45:A:LEU:O	7	0.1
(2,66)	1:160:A:TYR:H	1:152:A:THR:O	9	0.1
(2,16)	1:79:A:ASN:H	1:92:A:VAL:O	7	0.1
(1,1125)	1:133:A:GLN:HE21	1:130:A:MET:HE1	6	0.1
(1,1125)	1:133:A:GLN:HE21	1:130:A:MET:HE2	6	0.1
(1,1125)	1:133:A:GLN:HE21	1:130:A:MET:HE3	6	0.1
(1,1120)	1:123:A:GLN:HE21	1:122:A:LEU:HD21	9	0.1
(1,1120)	1:123:A:GLN:HE21	1:122:A:LEU:HD22	9	0.1
(1,1120)	1:123:A:GLN:HE21	1:122:A:LEU:HD23	9	0.1
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG21	10	0.1
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG22	10	0.1
(1,1116)	1:231:A:SER:H	1:230:A:VAL:HG23	10	0.1
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG11	2	0.1
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG12	2	0.1
(1,1115)	1:231:A:SER:H	1:230:A:VAL:HG13	2	0.1
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG21	1	0.1
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG22	1	0.1
(1,1099)	1:220:A:LEU:H	1:219:A:THR:HG23	1	0.1
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG21	2	0.1
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG22	2	0.1
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG23	2	0.1
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG21	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG22	8	0.1
(1,1083)	1:208:A:LYS:H	1:207:A:VAL:HG23	8	0.1
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD11	1	0.1
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD12	1	0.1
(1,1078)	1:207:A:VAL:H	1:49:A:ILE:HD13	1	0.1
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG11	4	0.1
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG12	4	0.1
(1,1069)	1:204:A:LYS:H	1:207:A:VAL:HG13	4	0.1
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG21	6	0.1
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG22	6	0.1
(1,975)	1:170:A:PHE:H	1:171:A:THR:HG23	6	0.1
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG21	7	0.1
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG22	7	0.1
(1,968)	1:163:A:GLU:H	1:171:A:THR:HG23	7	0.1
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD11	2	0.1
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD12	2	0.1
(1,962)	1:162:A:TRP:H	1:151:A:ILE:HD13	2	0.1
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG21	3	0.1
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG22	3	0.1
(1,956)	1:161:A:ALA:H	1:172:A:VAL:HG23	3	0.1
(1,936)	1:150:A:VAL:H	1:149:A:THR:HG21	3	0.1
(1,936)	1:150:A:VAL:H	1:149:A:THR:HG22	3	0.1
(1,936)	1:150:A:VAL:H	1:149:A:THR:HG23	3	0.1
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD11	1	0.1
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD12	1	0.1
(1,924)	1:145:A:ALA:H	1:188:A:LEU:HD13	1	0.1
(1,912)	1:142:A:TYR:H	1:143:A:LEU:HD21	6	0.1
(1,912)	1:142:A:TYR:H	1:143:A:LEU:HD22	6	0.1
(1,912)	1:142:A:TYR:H	1:143:A:LEU:HD23	6	0.1
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG11	2	0.1
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG12	2	0.1
(1,907)	1:141:A:ALA:H	1:148:A:VAL:HG13	2	0.1
(1,883)	1:127:A:ASP:H	1:121:A:ALA:HB1	3	0.1
(1,883)	1:127:A:ASP:H	1:121:A:ALA:HB2	3	0.1
(1,883)	1:127:A:ASP:H	1:121:A:ALA:HB3	3	0.1
(1,880)	1:126:A:ALA:H	1:122:A:LEU:HD11	6	0.1
(1,880)	1:126:A:ALA:H	1:122:A:LEU:HD12	6	0.1
(1,880)	1:126:A:ALA:H	1:122:A:LEU:HD13	6	0.1
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB1	3	0.1
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB2	3	0.1
(1,878)	1:125:A:GLY:H	1:124:A:ALA:HB3	3	0.1
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB1	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB2	5	0.1
(1,872)	1:123:A:GLN:H	1:121:A:ALA:HB3	5	0.1
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG11	1	0.1
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG12	1	0.1
(1,856)	1:104:A:ILE:H	1:172:A:VAL:HG13	1	0.1
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB1	7	0.1
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB2	7	0.1
(1,853)	1:104:A:ILE:H	1:101:A:ALA:HB3	7	0.1
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD11	2	0.1
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD12	2	0.1
(1,846)	1:94:A:THR:H	1:56:A:LEU:HD13	2	0.1
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG21	1	0.1
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG22	1	0.1
(1,820)	1:87:A:ARG:H	1:88:A:THR:HG23	1	0.1
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	6	0.1
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	6	0.1
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	6	0.1
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD11	8	0.1
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD12	8	0.1
(1,809)	1:83:A:ASN:H	1:89:A:LEU:HD13	8	0.1
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG21	8	0.1
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG22	8	0.1
(1,797)	1:80:A:LEU:H	1:219:A:THR:HG23	8	0.1
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG21	4	0.1
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG22	4	0.1
(1,786)	1:77:A:HIS:H	1:94:A:THR:HG23	4	0.1
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD21	5	0.1
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD22	5	0.1
(1,767)	1:63:A:SER:H	1:70:A:LEU:HD23	5	0.1
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD21	1	0.1
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD22	1	0.1
(1,761)	1:61:A:TYR:H	1:76:A:LEU:HD23	1	0.1
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD11	10	0.1
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD12	10	0.1
(1,749)	1:58:A:LYS:H	1:96:A:ILE:HD13	10	0.1
(1,721)	1:43:A:ILE:H	1:144:A:VAL:HG21	3	0.1
(1,721)	1:43:A:ILE:H	1:144:A:VAL:HG22	3	0.1
(1,721)	1:43:A:ILE:H	1:144:A:VAL:HG23	3	0.1
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD11	3	0.1
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD12	3	0.1
(1,715)	1:35:A:ASN:H	1:32:A:LEU:HD13	3	0.1
(1,705)	1:32:A:LEU:H	1:29:A:LEU:HD11	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:32:A:LEU:H	1:29:A:LEU:HD12	4	0.1
(1,705)	1:32:A:LEU:H	1:29:A:LEU:HD13	4	0.1
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB1	8	0.1
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB2	8	0.1
(1,699)	1:29:A:LEU:H	1:27:A:ALA:HB3	8	0.1
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG11	3	0.1
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG12	3	0.1
(1,688)	1:20:A:PHE:H	1:172:A:VAL:HG13	3	0.1
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG21	8	0.1
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG22	8	0.1
(1,681)	1:230:A:VAL:H	1:230:A:VAL:HG23	8	0.1
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG11	10	0.1
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG12	10	0.1
(1,672)	1:207:A:VAL:H	1:207:A:VAL:HG13	10	0.1
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG11	4	0.1
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG12	4	0.1
(1,659)	1:172:A:VAL:H	1:172:A:VAL:HG13	4	0.1
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG21	4	0.1
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG22	4	0.1
(1,653)	1:144:A:VAL:H	1:144:A:VAL:HG23	4	0.1
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD11	7	0.1
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD12	7	0.1
(1,635)	1:91:A:ILE:H	1:91:A:ILE:HD13	7	0.1
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB1	10	0.1
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB2	10	0.1
(1,553)	1:122:A:LEU:HD11	1:126:A:ALA:HB3	10	0.1
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB1	10	0.1
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB2	10	0.1
(1,553)	1:122:A:LEU:HD12	1:126:A:ALA:HB3	10	0.1
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB1	10	0.1
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB2	10	0.1
(1,553)	1:122:A:LEU:HD13	1:126:A:ALA:HB3	10	0.1
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG11	9	0.1
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG12	9	0.1
(1,533)	1:103:A:LEU:HD11	1:172:A:VAL:HG13	9	0.1
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG11	9	0.1
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG12	9	0.1
(1,533)	1:103:A:LEU:HD12	1:172:A:VAL:HG13	9	0.1
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG11	9	0.1
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG12	9	0.1
(1,533)	1:103:A:LEU:HD13	1:172:A:VAL:HG13	9	0.1
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD11	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD12	7	0.1
(1,528)	1:103:A:LEU:HD11	1:107:A:LEU:HD13	7	0.1
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD11	7	0.1
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD12	7	0.1
(1,528)	1:103:A:LEU:HD12	1:107:A:LEU:HD13	7	0.1
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD11	7	0.1
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD12	7	0.1
(1,528)	1:103:A:LEU:HD13	1:107:A:LEU:HD13	7	0.1
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD11	9	0.1
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD12	9	0.1
(1,510)	1:90:A:THR:HG21	1:187:A:ILE:HD13	9	0.1
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD11	9	0.1
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD12	9	0.1
(1,510)	1:90:A:THR:HG22	1:187:A:ILE:HD13	9	0.1
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD11	9	0.1
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD12	9	0.1
(1,510)	1:90:A:THR:HG23	1:187:A:ILE:HD13	9	0.1
(1,502)	1:89:A:LEU:HD11	1:203:A:ILE:HD11	2	0.1
(1,502)	1:89:A:LEU:HD11	1:203:A:ILE:HD12	2	0.1
(1,502)	1:89:A:LEU:HD11	1:203:A:ILE:HD13	2	0.1
(1,502)	1:89:A:LEU:HD12	1:203:A:ILE:HD11	2	0.1
(1,502)	1:89:A:LEU:HD12	1:203:A:ILE:HD12	2	0.1
(1,502)	1:89:A:LEU:HD12	1:203:A:ILE:HD13	2	0.1
(1,502)	1:89:A:LEU:HD13	1:203:A:ILE:HD11	2	0.1
(1,502)	1:89:A:LEU:HD13	1:203:A:ILE:HD12	2	0.1
(1,502)	1:89:A:LEU:HD13	1:203:A:ILE:HD13	2	0.1
(1,501)	1:89:A:LEU:HD11	1:198:A:LEU:HD21	4	0.1
(1,501)	1:89:A:LEU:HD11	1:198:A:LEU:HD22	4	0.1
(1,501)	1:89:A:LEU:HD11	1:198:A:LEU:HD23	4	0.1
(1,501)	1:89:A:LEU:HD12	1:198:A:LEU:HD21	4	0.1
(1,501)	1:89:A:LEU:HD12	1:198:A:LEU:HD22	4	0.1
(1,501)	1:89:A:LEU:HD12	1:198:A:LEU:HD23	4	0.1
(1,501)	1:89:A:LEU:HD13	1:198:A:LEU:HD21	4	0.1
(1,501)	1:89:A:LEU:HD13	1:198:A:LEU:HD22	4	0.1
(1,501)	1:89:A:LEU:HD13	1:198:A:LEU:HD23	4	0.1
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD11	10	0.1
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD12	10	0.1
(1,493)	1:80:A:LEU:HD11	1:220:A:LEU:HD13	10	0.1
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD11	10	0.1
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD12	10	0.1
(1,493)	1:80:A:LEU:HD12	1:220:A:LEU:HD13	10	0.1
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD11	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD12	10	0.1
(1,493)	1:80:A:LEU:HD13	1:220:A:LEU:HD13	10	0.1
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD11	10	0.1
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD12	10	0.1
(1,476)	1:49:A:ILE:HD11	1:218:A:ILE:HD13	10	0.1
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD11	10	0.1
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD12	10	0.1
(1,476)	1:49:A:ILE:HD12	1:218:A:ILE:HD13	10	0.1
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD11	10	0.1
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD12	10	0.1
(1,476)	1:49:A:ILE:HD13	1:218:A:ILE:HD13	10	0.1
(1,455)	1:45:A:LEU:HD21	1:80:A:LEU:HD21	8	0.1
(1,455)	1:45:A:LEU:HD21	1:80:A:LEU:HD22	8	0.1
(1,455)	1:45:A:LEU:HD21	1:80:A:LEU:HD23	8	0.1
(1,455)	1:45:A:LEU:HD22	1:80:A:LEU:HD21	8	0.1
(1,455)	1:45:A:LEU:HD22	1:80:A:LEU:HD22	8	0.1
(1,455)	1:45:A:LEU:HD22	1:80:A:LEU:HD23	8	0.1
(1,455)	1:45:A:LEU:HD23	1:80:A:LEU:HD21	8	0.1
(1,455)	1:45:A:LEU:HD23	1:80:A:LEU:HD22	8	0.1
(1,455)	1:45:A:LEU:HD23	1:80:A:LEU:HD23	8	0.1
(1,451)	1:45:A:LEU:HD11	1:207:A:VAL:HG21	1	0.1
(1,451)	1:45:A:LEU:HD11	1:207:A:VAL:HG22	1	0.1
(1,451)	1:45:A:LEU:HD11	1:207:A:VAL:HG23	1	0.1
(1,451)	1:45:A:LEU:HD12	1:207:A:VAL:HG21	1	0.1
(1,451)	1:45:A:LEU:HD12	1:207:A:VAL:HG22	1	0.1
(1,451)	1:45:A:LEU:HD12	1:207:A:VAL:HG23	1	0.1
(1,451)	1:45:A:LEU:HD13	1:207:A:VAL:HG21	1	0.1
(1,451)	1:45:A:LEU:HD13	1:207:A:VAL:HG22	1	0.1
(1,451)	1:45:A:LEU:HD13	1:207:A:VAL:HG23	1	0.1
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD11	6	0.1
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD12	6	0.1
(1,426)	1:30:A:MET:HE1	1:34:A:ILE:HD13	6	0.1
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD11	6	0.1
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD12	6	0.1
(1,426)	1:30:A:MET:HE2	1:34:A:ILE:HD13	6	0.1
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD11	6	0.1
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD12	6	0.1
(1,426)	1:30:A:MET:HE3	1:34:A:ILE:HD13	6	0.1
(1,413)	1:29:A:LEU:HD11	1:115:A:THR:HG21	6	0.1
(1,413)	1:29:A:LEU:HD11	1:115:A:THR:HG22	6	0.1
(1,413)	1:29:A:LEU:HD11	1:115:A:THR:HG23	6	0.1
(1,413)	1:29:A:LEU:HD12	1:115:A:THR:HG21	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:29:A:LEU:HD12	1:115:A:THR:HG22	6	0.1
(1,413)	1:29:A:LEU:HD12	1:115:A:THR:HG23	6	0.1
(1,413)	1:29:A:LEU:HD13	1:115:A:THR:HG21	6	0.1
(1,413)	1:29:A:LEU:HD13	1:115:A:THR:HG22	6	0.1
(1,413)	1:29:A:LEU:HD13	1:115:A:THR:HG23	6	0.1
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD21	5	0.1
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD22	5	0.1
(1,411)	1:29:A:LEU:HD11	1:32:A:LEU:HD23	5	0.1
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD21	5	0.1
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD22	5	0.1
(1,411)	1:29:A:LEU:HD12	1:32:A:LEU:HD23	5	0.1
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD21	5	0.1
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD22	5	0.1
(1,411)	1:29:A:LEU:HD13	1:32:A:LEU:HD23	5	0.1
(1,366)	1:163:A:GLU:H	1:171:A:THR:H	5	0.1
(1,343)	1:114:A:GLY:H	1:118:A:PHE:H	7	0.1
(1,341)	1:95:A:GLY:H	1:184:A:THR:H	2	0.1
(1,337)	1:89:A:LEU:H	1:190:A:LEU:H	5	0.1
(1,270)	1:104:A:ILE:H	1:107:A:LEU:H	3	0.1
(1,242)	1:223:A:GLU:H	1:225:A:GLU:H	2	0.1
(1,242)	1:223:A:GLU:H	1:225:A:GLU:H	10	0.1
(1,200)	1:123:A:GLN:H	1:125:A:GLY:H	1	0.1
(1,50)	1:87:A:ARG:H	1:88:A:THR:H	5	0.1
(1,35)	1:69:A:LYS:H	1:70:A:LEU:H	6	0.1

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

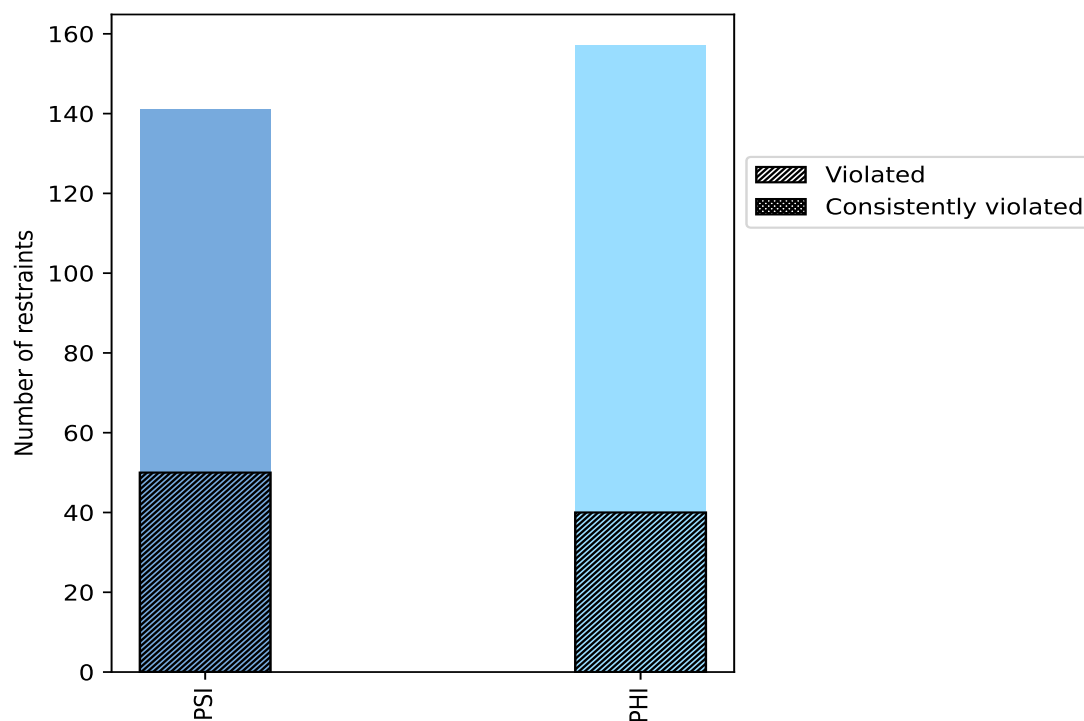
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	141	47.3	50	35.5	16.8	0	0.0	0.0
PHI	157	52.7	40	25.5	13.4	0	0.0	0.0
Total	298	100.0	90	30.2	30.2	0	0.0	0.0

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

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



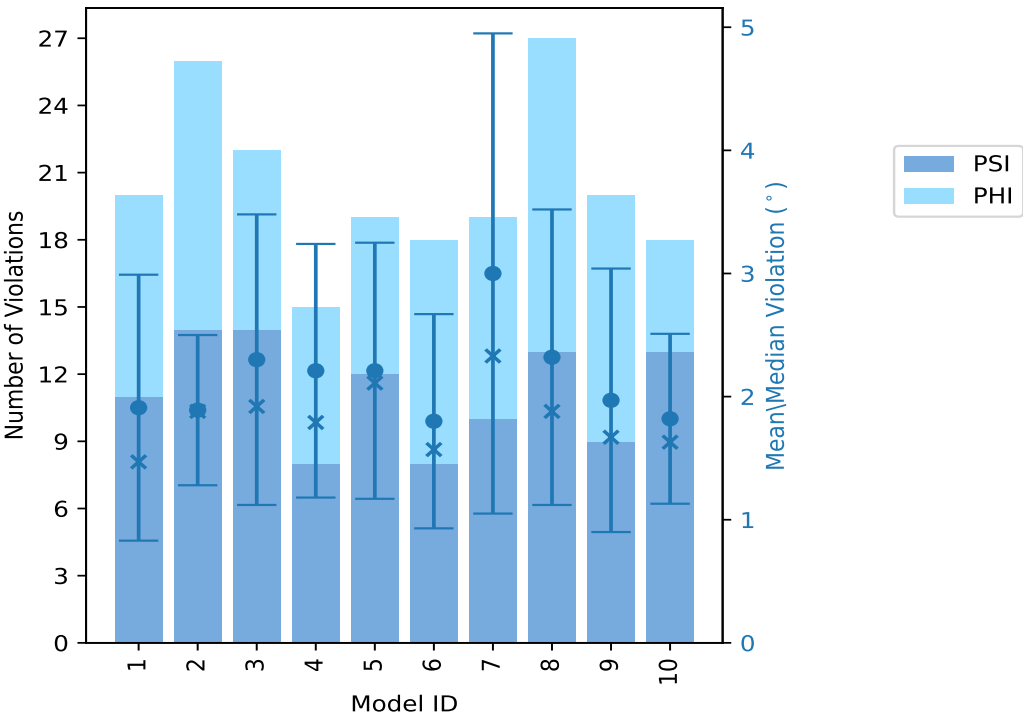
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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 (°)
	PSI	PHI	Total				
1	11	9	20	1.91	5.46	1.08	1.47
2	14	12	26	1.89	4.03	0.61	1.88
3	14	8	22	2.3	5.44	1.18	1.92
4	8	7	15	2.21	4.32	1.03	1.79
5	12	7	19	2.21	4.89	1.04	2.11
6	8	10	18	1.8	3.96	0.87	1.57
7	10	9	19	3.0	8.38	1.95	2.33
8	13	14	27	2.32	6.01	1.2	1.88
9	9	11	20	1.97	4.78	1.07	1.67
10	13	5	18	1.82	3.59	0.69	1.63

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

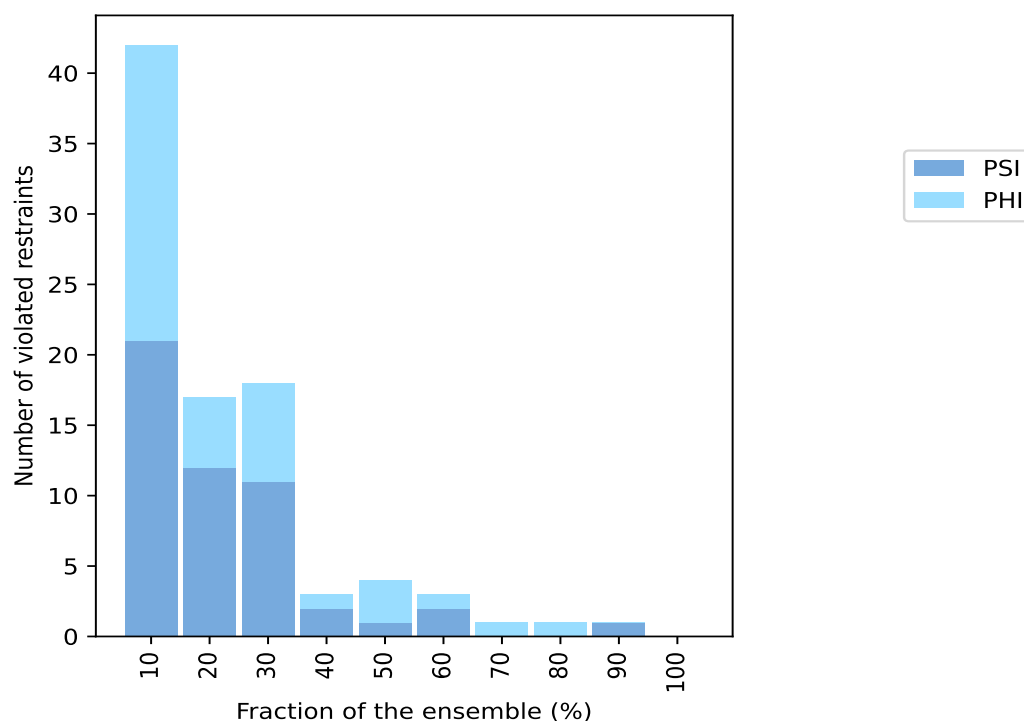
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
21	21	42	1	10.0
12	5	17	2	20.0
11	7	18	3	30.0
2	1	3	4	40.0
1	3	4	5	50.0
2	1	3	6	60.0
0	1	1	7	70.0
0	1	1	8	80.0
1	0	1	9	90.0
0	0	0	10	100.0

¹ Number of models with violations

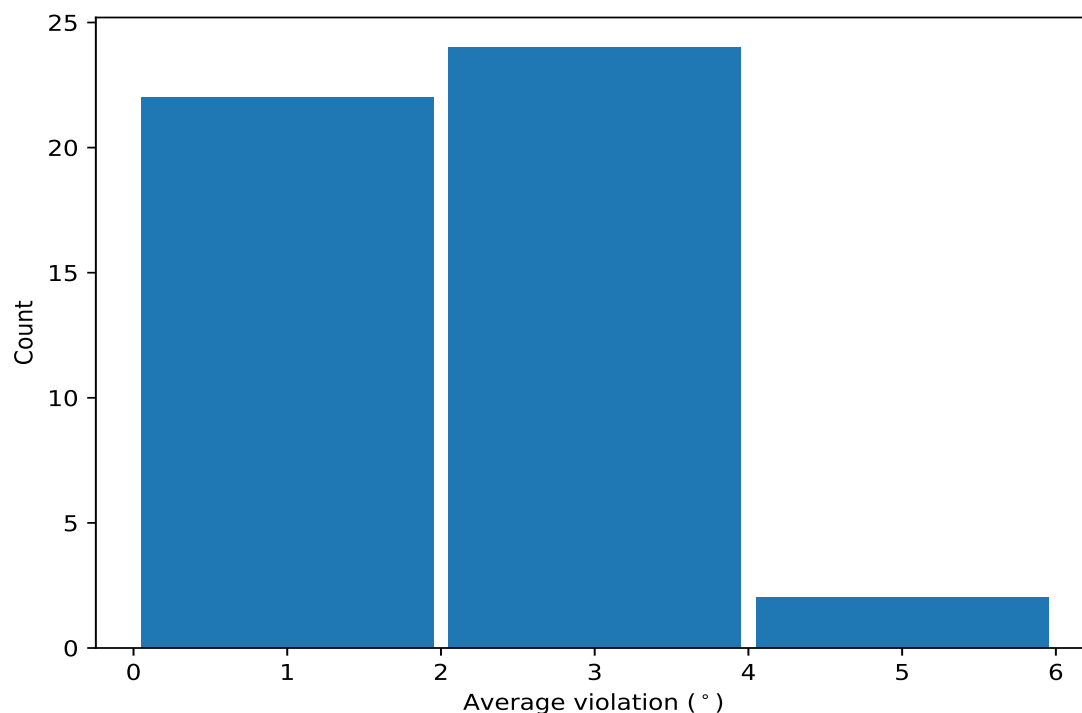
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	9	2.01	1.01	1.41
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	8	2.58	1.62	1.78
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	7	2.85	1.22	3.09
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	6	2.58	1.71	1.68
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	6	2.15	0.57	1.88
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	6	1.78	0.46	1.59
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	5	2.61	0.72	2.41
(1,137)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:ASP:N	5	2.42	0.98	2.6
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	5	2.13	0.54	2.29
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	5	1.76	0.74	1.52
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	4	2.53	0.62	2.38
(1,199)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	4	2.11	0.93	1.82
(1,292)	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	1:233:A:ASP:N	4	1.44	0.32	1.3

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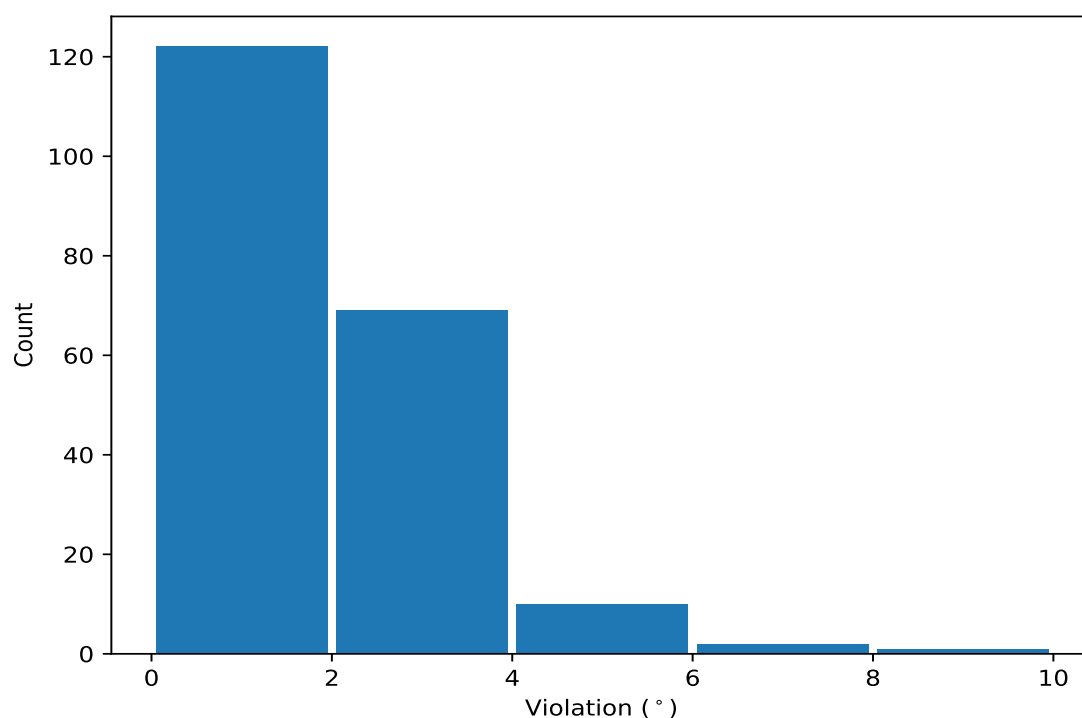
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,72)	1:70:A:LEU:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	3	4.67	0.66	4.71
(1,180)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	3	3.58	2.48	1.97
(1,73)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:SER:N	3	2.95	1.04	2.71
(1,196)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	3	2.36	0.89	1.85
(1,179)	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1:156:A:ASP:N	3	2.31	1.01	2.47
(1,70)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:LYS:N	3	2.23	0.26	2.41
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	3	2.07	0.29	2.13
(1,138)	1:126:A:ALA:C	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	3	2.05	0.66	2.41
(1,175)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:HIS:N	3	1.98	0.99	1.28
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	3	1.83	0.56	2.11
(1,123)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	3	1.8	0.92	1.27
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	3	1.79	0.49	1.76
(1,207)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	3	1.65	0.46	1.75
(1,215)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	3	1.56	0.34	1.33
(1,269)	1:218:A:ILE:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	3	1.55	0.38	1.55
(1,85)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	3	1.37	0.03	1.36
(1,22)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	3	1.27	0.3	1.12
(1,210)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	3	1.25	0.31	1.03
(1,173)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:LYS:N	2	4.19	0.6	4.19
(1,212)	1:182:A:ARG:N	1:182:A:ARG:CA	1:182:A:ARG:C	1:183:A:GLY:N	2	3.41	0.15	3.41
(1,93)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	2	3.32	1.56	3.32
(1,71)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	2	3.22	0.53	3.22
(1,1)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	2	2.59	1.09	2.59
(1,154)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:TYR:N	2	2.56	0.36	2.56
(1,177)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	2	2.34	1.27	2.34
(1,225)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	2	2.26	1.04	2.26
(1,286)	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	1:230:A:VAL:N	2	1.98	0.26	1.98
(1,86)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	2	1.78	0.25	1.78
(1,262)	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	1:215:A:GLY:N	2	1.54	0.38	1.54
(1,78)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:ASN:N	2	1.43	0.16	1.43
(1,76)	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1:78:A:ILE:N	2	1.38	0.16	1.38
(1,296)	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	1:235:A:ALA:N	2	1.33	0.29	1.33
(1,284)	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	1:227:A:ASP:N	2	1.19	0.17	1.19
(1,204)	1:173:A:ARG:C	1:174:A:THR:N	1:174:A:THR:CA	1:174:A:THR:C	2	1.12	0.04	1.12
(1,287)	1:229:A:GLU:C	1:230:A:VAL:N	1:230:A:VAL:CA	1:230:A:VAL:C	2	1.11	0.09	1.11

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,283)	1:225:A:GLU:C	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	7	8.38
(1,180)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	7	7.08
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	8	6.01
(1,72)	1:70:A:LEU:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1	5.46
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	3	5.44
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	8	5.04
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	7	5.02
(1,93)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	5	4.89
(1,173)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:LYS:N	9	4.78
(1,72)	1:70:A:LEU:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	9	4.71
(1,156)	1:142:A:TYR:N	1:142:A:TYR:CA	1:142:A:TYR:C	1:143:A:LEU:N	3	4.64
(1,73)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:SER:N	4	4.32
(1,137)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:ASP:N	2	4.03
(1,105)	1:95:A:GLY:C	1:96:A:ILE:N	1:96:A:ILE:CA	1:96:A:ILE:C	7	3.97
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	6	3.96
(1,72)	1:70:A:LEU:C	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	4	3.84
(1,71)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	4	3.75
(1,1)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	3	3.68
(1,199)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	7	3.65
(1,196)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1	3.62
(1,177)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	7	3.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	10	3.59
(1,173)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:LYS:N	5	3.59
(1,212)	1:182:A:ARG:N	1:182:A:ARG:CA	1:182:A:ARG:C	1:183:A:GLY:N	8	3.56
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	7	3.5
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	9	3.47
(1,179)	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1:156:A:ASP:N	3	3.46
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	5	3.44
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	5	3.41
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	8	3.4
(1,175)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:HIS:N	8	3.38
(1,225)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	6	3.3
(1,212)	1:182:A:ARG:N	1:182:A:ARG:CA	1:182:A:ARG:C	1:183:A:GLY:N	3	3.26
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	8	3.2
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	7	3.16
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	6	3.09
(1,123)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	8	3.09
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	3	2.98
(1,29)	1:43:A:ILE:C	1:44:A:PHE:N	1:44:A:PHE:CA	1:44:A:PHE:C	4	2.96
(1,154)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:TYR:N	8	2.92
(1,67)	1:65:A:THR:C	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	4	2.92
(1,201)	1:172:A:VAL:N	1:172:A:VAL:CA	1:172:A:VAL:C	1:173:A:ARG:N	5	2.88
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	6	2.88
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1	2.84
(1,73)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:SER:N	1	2.71
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	8	2.71
(1,87)	1:82:A:PRO:C	1:83:A:ASN:N	1:83:A:ASN:CA	1:83:A:ASN:C	5	2.7
(1,71)	1:69:A:LYS:C	1:70:A:LEU:N	1:70:A:LEU:CA	1:70:A:LEU:C	8	2.69
(1,137)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:ASP:N	10	2.66
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1	2.64
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	3	2.63
(1,23)	1:34:A:ILE:C	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	2	2.62
(1,138)	1:126:A:ALA:C	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	2	2.61
(1,137)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:ASP:N	3	2.6
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	10	2.59
(1,179)	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1:156:A:ASP:N	10	2.47
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	7	2.44
(1,70)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:LYS:N	1	2.43
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	9	2.41
(1,138)	1:126:A:ALA:C	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	3	2.41
(1,70)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:LYS:N	5	2.41
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	2	2.41
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	10	2.39
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	10	2.38
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	5	2.35
(1,104)	1:93:A:ASP:C	1:94:A:THR:N	1:94:A:THR:CA	1:94:A:THR:C	8	2.35
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	7	2.33
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	5	2.31
(1,183)	1:159:A:GLN:N	1:159:A:GLN:CA	1:159:A:GLN:C	1:160:A:TYR:N	3	2.29
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	2	2.29
(1,286)	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	1:230:A:VAL:N	2	2.25
(1,154)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:TYR:N	2	2.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,274)	1:221:A:PHE:N	1:221:A:PHE:CA	1:221:A:PHE:C	1:222:A:VAL:N	8	2.16
(1,207)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	2	2.16
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	7	2.13
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	4	2.12
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	5	2.11
(1,169)	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	1:151:A:ILE:N	2	2.06
(1,215)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	8	2.05
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	9	2.03
(1,86)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	2	2.03
(1,269)	1:218:A:ILE:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	9	2.01
(1,292)	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	1:233:A:ASP:N	3	1.99
(1,180)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1	1.97
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	2	1.93
(1,262)	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	1:215:A:GLY:N	2	1.93
(1,220)	1:186:A:VAL:N	1:186:A:VAL:CA	1:186:A:VAL:C	1:187:A:ILE:N	2	1.92
(1,270)	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	1:220:A:LEU:N	8	1.88
(1,75)	1:76:A:LEU:C	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	9	1.87
(1,70)	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	1:69:A:LYS:N	6	1.86
(1,196)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	3	1.85
(1,157)	1:142:A:TYR:C	1:143:A:LEU:N	1:143:A:LEU:CA	1:143:A:LEU:C	2	1.85
(1,199)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	5	1.82
(1,199)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	10	1.82
(1,73)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:SER:N	9	1.81
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	7	1.8
(1,280)	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	1:225:A:GLU:N	4	1.79
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	4	1.79
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	6	1.78
(1,93)	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	1:89:A:LEU:N	3	1.76
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	8	1.76
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	2	1.75
(1,207)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	5	1.75
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	10	1.73
(1,286)	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	1:230:A:VAL:N	7	1.72
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	4	1.71
(1,210)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	3	1.69
(1,189)	1:162:A:TRP:N	1:162:A:TRP:CA	1:162:A:TRP:C	1:163:A:GLU:N	9	1.69
(1,180)	1:156:A:ASP:C	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	9	1.68
(1,22)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	3	1.68
(1,214)	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	1:184:A:THR:N	8	1.67
(1,57)	1:59:A:ILE:C	1:60:A:ARG:N	1:60:A:ARG:CA	1:60:A:ARG:C	6	1.66
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	9	1.66
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	10	1.64
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	2	1.63
(1,196)	1:169:A:SER:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	10	1.62
(1,296)	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	1:235:A:ALA:N	1	1.61
(1,66)	1:64:A:LEU:N	1:64:A:LEU:CA	1:64:A:LEU:C	1:65:A:THR:N	6	1.61
(1,291)	1:231:A:SER:C	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	8	1.6
(1,271)	1:219:A:THR:C	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	6	1.59
(1,78)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:ASN:N	7	1.59
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	2	1.59
(1,261)	1:213:A:PHE:C	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	8	1.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,269)	1:218:A:ILE:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	6	1.55
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	1	1.55
(1,194)	1:168:A:GLY:C	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	8	1.55
(1,176)	1:153:A:LYS:C	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	7	1.54
(1,160)	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	1:146:A:GLU:N	2	1.54
(1,76)	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1:78:A:ILE:N	10	1.54
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1	1.52
(1,86)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:ASN:N	4	1.52
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	2	1.5
(1,205)	1:174:A:THR:N	1:174:A:THR:CA	1:174:A:THR:C	1:175:A:ASP:N	10	1.5
(1,137)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:ASP:N	9	1.5
(1,1)	1:17:A:VAL:C	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	8	1.5
(1,218)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:VAL:N	2	1.49
(1,295)	1:233:A:ASP:C	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	2	1.46
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	9	1.46
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	4	1.46
(1,193)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:SER:N	8	1.44
(1,197)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:THR:N	1	1.42
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	7	1.41
(1,85)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1	1.41
(1,147)	1:132:A:GLY:C	1:133:A:GLN:N	1:133:A:GLN:CA	1:133:A:GLN:C	9	1.39
(1,284)	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	1:227:A:ASP:N	7	1.36
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	3	1.36
(1,85)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	8	1.36
(1,292)	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	1:233:A:ASP:N	8	1.35
(1,85)	1:81:A:ILE:C	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	6	1.35
(1,19)	1:32:A:LEU:C	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	5	1.35
(1,215)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	7	1.33
(1,215)	1:183:A:GLY:C	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	5	1.31
(1,198)	1:170:A:PHE:C	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	2	1.31
(1,279)	1:223:A:GLU:C	1:224:A:LYS:N	1:224:A:LYS:CA	1:224:A:LYS:C	9	1.29
(1,137)	1:126:A:ALA:N	1:126:A:ALA:CA	1:126:A:ALA:C	1:127:A:ASP:N	4	1.29
(1,10)	1:22:A:PHE:N	1:22:A:PHE:CA	1:22:A:PHE:C	1:23:A:GLN:N	4	1.29
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	4	1.28
(1,175)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:HIS:N	6	1.28
(1,175)	1:153:A:LYS:N	1:153:A:LYS:CA	1:153:A:LYS:C	1:154:A:HIS:N	5	1.27
(1,123)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	1	1.27
(1,78)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:ASN:N	3	1.27
(1,292)	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	1:233:A:ASP:N	10	1.25
(1,25)	1:38:A:TYR:C	1:39:A:SER:N	1:39:A:SER:CA	1:39:A:SER:C	5	1.25
(1,225)	1:188:A:LEU:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	2	1.22
(1,216)	1:184:A:THR:N	1:184:A:THR:CA	1:184:A:THR:C	1:185:A:LYS:N	10	1.22
(1,76)	1:77:A:HIS:N	1:77:A:HIS:CA	1:77:A:HIS:C	1:78:A:ILE:N	1	1.22
(1,285)	1:228:A:LYS:C	1:229:A:GLU:N	1:229:A:GLU:CA	1:229:A:GLU:C	9	1.21
(1,287)	1:229:A:GLU:C	1:230:A:VAL:N	1:230:A:VAL:CA	1:230:A:VAL:C	3	1.2
(1,2)	1:18:A:GLU:N	1:18:A:GLU:CA	1:18:A:GLU:C	1:19:A:THR:N	3	1.2
(1,292)	1:232:A:ASP:N	1:232:A:ASP:CA	1:232:A:ASP:C	1:233:A:ASP:N	1	1.19
(1,64)	1:63:A:SER:N	1:63:A:SER:CA	1:63:A:SER:C	1:64:A:LEU:N	6	1.19
(1,7)	1:20:A:PHE:C	1:21:A:ALA:N	1:21:A:ALA:CA	1:21:A:ALA:C	2	1.19
(1,199)	1:171:A:THR:N	1:171:A:THR:CA	1:171:A:THR:C	1:172:A:VAL:N	9	1.17
(1,282)	1:225:A:GLU:N	1:225:A:GLU:CA	1:225:A:GLU:C	1:226:A:ARG:N	4	1.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,262)	1:214:A:ILE:N	1:214:A:ILE:CA	1:214:A:ILE:C	1:215:A:GLY:N	8	1.16
(1,204)	1:173:A:ARG:C	1:174:A:THR:N	1:174:A:THR:CA	1:174:A:THR:C	8	1.16
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	6	1.16
(1,122)	1:110:A:ILE:C	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	2	1.15
(1,290)	1:231:A:SER:N	1:231:A:SER:CA	1:231:A:SER:C	1:232:A:ASP:N	5	1.14
(1,24)	1:35:A:ASN:N	1:35:A:ASN:CA	1:35:A:ASN:C	1:36:A:GLU:N	10	1.14
(1,277)	1:222:A:VAL:C	1:223:A:GLU:N	1:223:A:GLU:CA	1:223:A:GLU:C	1	1.12
(1,195)	1:169:A:SER:N	1:169:A:SER:CA	1:169:A:SER:C	1:170:A:PHE:N	1	1.12
(1,138)	1:126:A:ALA:C	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	9	1.12
(1,22)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	10	1.12
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	9	1.11
(1,269)	1:218:A:ILE:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	3	1.09
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	5	1.09
(1,266)	1:217:A:PRO:N	1:217:A:PRO:CA	1:217:A:PRO:C	1:218:A:ILE:N	1	1.07
(1,204)	1:173:A:ARG:C	1:174:A:THR:N	1:174:A:THR:CA	1:174:A:THR:C	1	1.07
(1,177)	1:154:A:HIS:N	1:154:A:HIS:CA	1:154:A:HIS:C	1:155:A:ASN:N	3	1.06
(1,233)	1:192:A:GLU:C	1:193:A:ASP:N	1:193:A:ASP:CA	1:193:A:ASP:C	8	1.05
(1,207)	1:175:A:ASP:N	1:175:A:ASP:CA	1:175:A:ASP:C	1:176:A:THR:N	9	1.05
(1,181)	1:157:A:ASP:N	1:157:A:ASP:CA	1:157:A:ASP:C	1:158:A:GLU:N	6	1.05
(1,296)	1:234:A:GLU:N	1:234:A:GLU:CA	1:234:A:GLU:C	1:235:A:ALA:N	7	1.04
(1,184)	1:159:A:GLN:C	1:160:A:TYR:N	1:160:A:TYR:CA	1:160:A:TYR:C	2	1.04
(1,213)	1:182:A:ARG:C	1:183:A:GLY:N	1:183:A:GLY:CA	1:183:A:GLY:C	6	1.03
(1,210)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	1	1.03
(1,123)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:LYS:N	10	1.03
(1,287)	1:229:A:GLU:C	1:230:A:VAL:N	1:230:A:VAL:CA	1:230:A:VAL:C	6	1.02
(1,284)	1:226:A:ARG:N	1:226:A:ARG:CA	1:226:A:ARG:C	1:227:A:ASP:N	10	1.02
(1,232)	1:192:A:GLU:N	1:192:A:GLU:CA	1:192:A:GLU:C	1:193:A:ASP:N	3	1.02
(1,210)	1:180:A:MET:N	1:180:A:MET:CA	1:180:A:MET:C	1:181:A:GLY:N	8	1.02
(1,179)	1:155:A:ASN:N	1:155:A:ASN:CA	1:155:A:ASN:C	1:156:A:ASP:N	6	1.01
(1,22)	1:34:A:ILE:N	1:34:A:ILE:CA	1:34:A:ILE:C	1:35:A:ASN:N	5	1.0