



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 05:17 PM EST

PDB ID : 2LQU  
BMRB ID : 18329  
Title : Structure of decorbin-binding protein A from *Borrelia burgdorferi*  
Authors : Wang, X.  
Deposited on : 2012-03-14

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

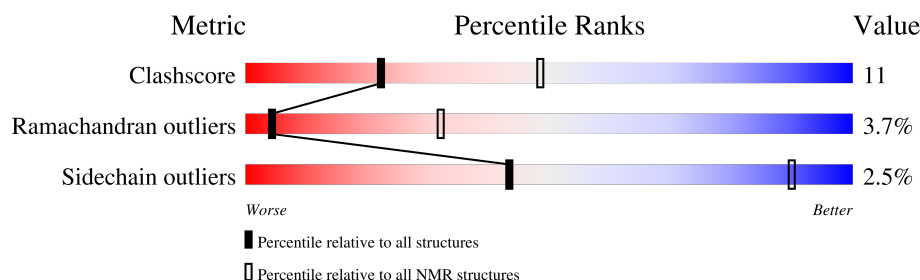
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 78%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	168	 62% 12% • 26%

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:30-A:55, A:75-A:103, A:109-A:178 (125)	0.84	4

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

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

The models can be grouped into 1 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2630 atoms, of which 1333 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Decorin-binding protein A.

Mol	Chain	Residues	Atoms						Trace
1	A	168	Total	C	H	N	O	S	0
			2630	809	1333	220	262	6	

There is a discrepancy between the modelled and reference sequences:

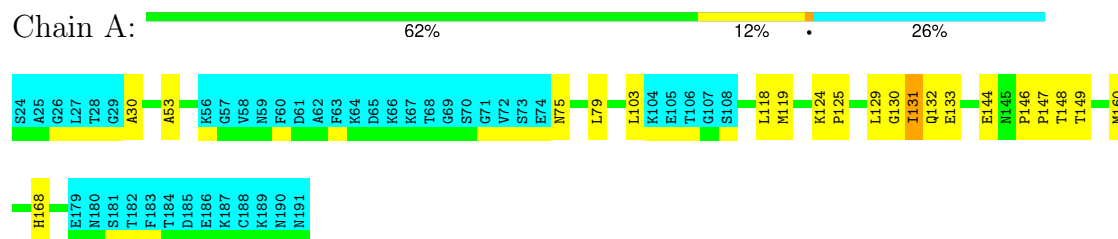
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	CYS	engineered mutation	UNP O50917

## 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: Decorin-binding protein A

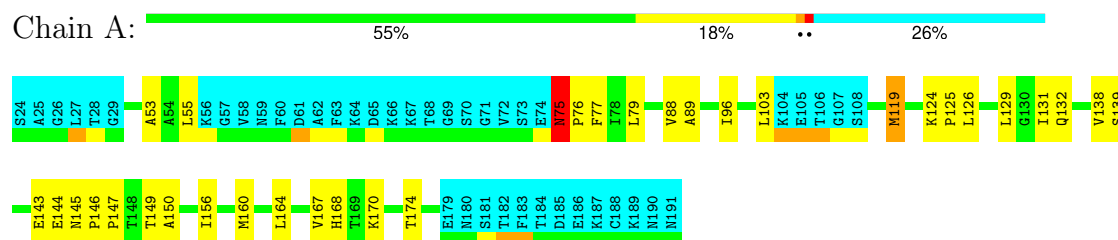


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

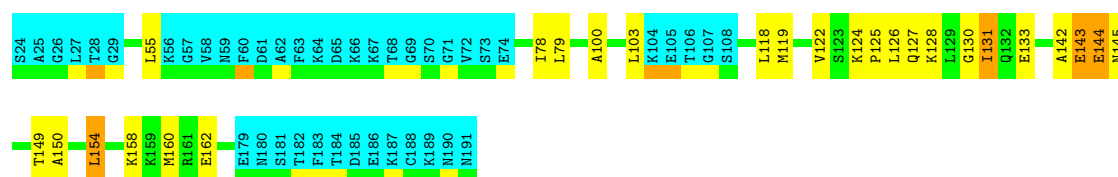
- Molecule 1: Decorin-binding protein A



#### 4.2.2 Score per residue for model 2

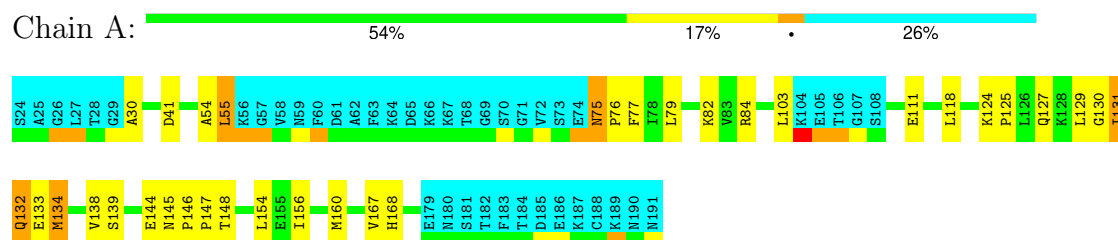
- Molecule 1: Decorin-binding protein A





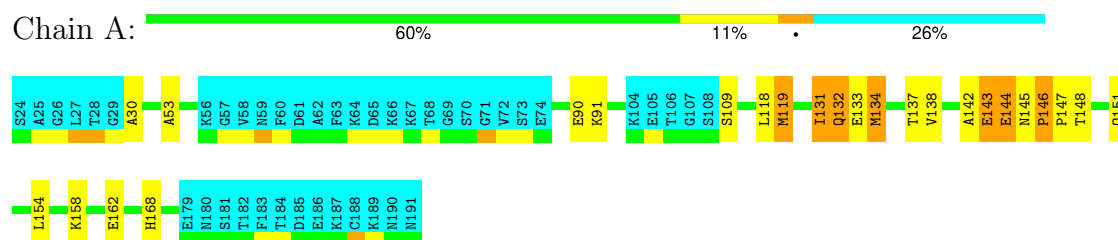
### 4.2.3 Score per residue for model 3

- Molecule 1: Decorin-binding protein A



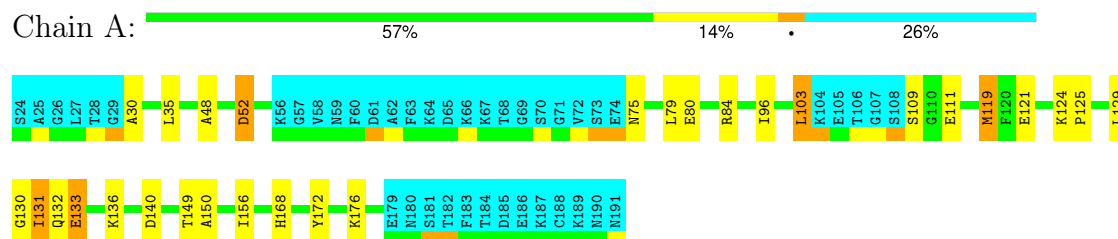
### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Decorin-binding protein A



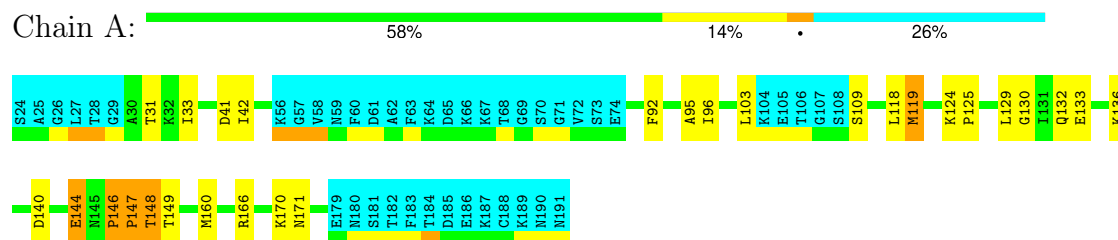
### 4.2.5 Score per residue for model 5

- Molecule 1: Decorin-binding protein A



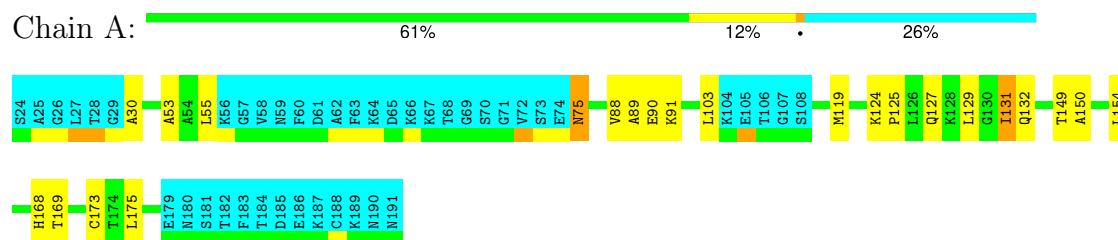
### 4.2.6 Score per residue for model 6

- Molecule 1: Decorin-binding protein A



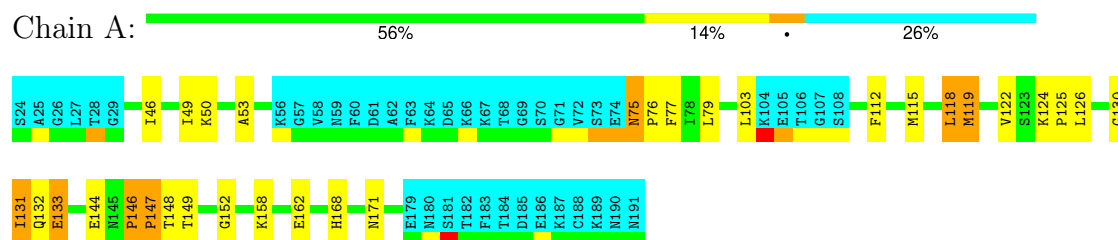
#### 4.2.7 Score per residue for model 7

- Molecule 1: Decorin-binding protein A



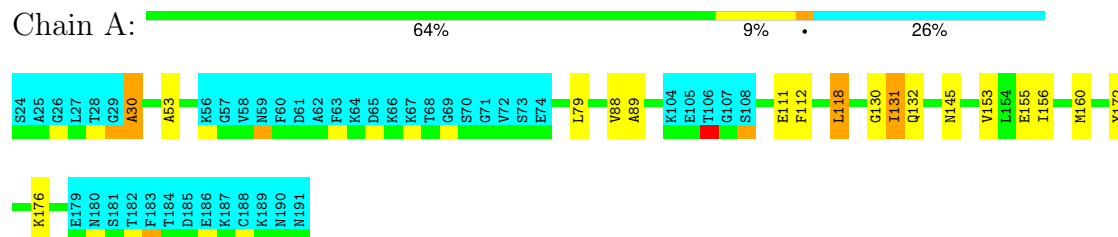
#### 4.2.8 Score per residue for model 8

- Molecule 1: Decorin-binding protein A



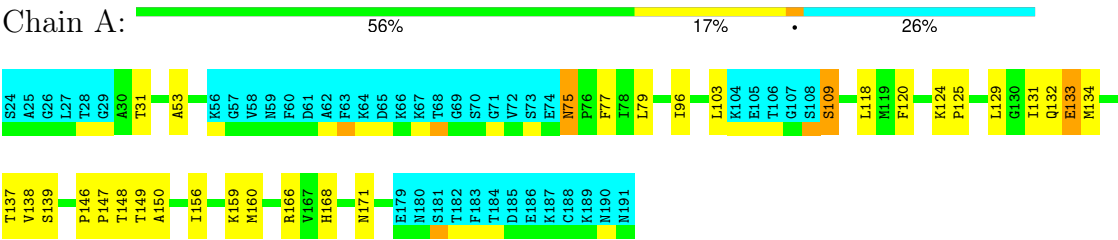
#### 4.2.9 Score per residue for model 9

- Molecule 1: Decorin-binding protein A



4.2.10 Score per residue for model 10

● Molecule 1: Decorin-binding protein A





## 5 Refinement protocol and experimental data overview

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

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	

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	1725
Number of shifts mapped to atoms	1725
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	981	1032	1031	22±6
All	All	9810	10320	10310	225

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ILE:O	1:A:132:GLN:O	0.92	1.88	3	1
1:A:131:ILE:HG22	1:A:132:GLN:H	0.89	1.24	9	3
1:A:131:ILE:HD12	1:A:131:ILE:N	0.75	1.95	2	2
1:A:156:ILE:HG22	1:A:160:MET:SD	0.70	2.27	10	2
1:A:131:ILE:HG22	1:A:131:ILE:O	0.66	1.91	10	1
1:A:164:LEU:O	1:A:167:VAL:HG22	0.63	1.93	1	1
1:A:79:LEU:HD22	1:A:79:LEU:N	0.62	2.08	3	1
1:A:149:THR:HG22	1:A:150:ALA:N	0.60	2.11	1	4
1:A:131:ILE:HG22	1:A:132:GLN:N	0.59	2.12	4	2
1:A:130:GLY:O	1:A:131:ILE:C	0.59	2.40	5	3
1:A:132:GLN:O	1:A:134:MET:N	0.58	2.37	3	1
1:A:143:GLU:O	1:A:145:ASN:N	0.58	2.36	4	2
1:A:130:GLY:C	1:A:131:ILE:HD12	0.57	2.20	9	1
1:A:75:ASN:HD22	1:A:75:ASN:N	0.57	1.98	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:TYR:CE2	1:A:176:LYS:NZ	0.57	2.73	5	1
1:A:120:PHE:CZ	1:A:124:LYS:NZ	0.57	2.71	10	1
1:A:131:ILE:CG2	1:A:132:GLN:H	0.56	2.05	9	1
1:A:131:ILE:N	1:A:131:ILE:CD1	0.56	2.68	2	1
1:A:79:LEU:N	1:A:79:LEU:CD2	0.55	2.69	3	1
1:A:172:TYR:CZ	1:A:176:LYS:NZ	0.55	2.74	5	2
1:A:146:PRO:O	1:A:148:THR:N	0.55	2.40	8	5
1:A:119:MET:SD	1:A:160:MET:SD	0.54	3.05	2	1
1:A:33:ILE:HD12	1:A:33:ILE:N	0.54	2.18	6	1
1:A:92:PHE:O	1:A:95:ALA:HB3	0.53	2.03	6	1
1:A:131:ILE:O	1:A:132:GLN:C	0.53	2.47	10	2
1:A:156:ILE:HD12	1:A:156:ILE:N	0.53	2.18	1	3
1:A:146:PRO:C	1:A:148:THR:H	0.53	2.07	6	1
1:A:54:ALA:O	1:A:55:LEU:C	0.53	2.46	3	1
1:A:122:VAL:O	1:A:126:LEU:HD23	0.52	2.04	2	2
1:A:75:ASN:ND2	1:A:75:ASN:N	0.52	2.58	1	1
1:A:35:LEU:HD22	1:A:35:LEU:N	0.51	2.20	5	1
1:A:154:LEU:HD22	1:A:154:LEU:N	0.51	2.20	3	1
1:A:75:ASN:N	1:A:75:ASN:ND2	0.51	2.57	3	1
1:A:75:ASN:C	1:A:77:PHE:H	0.50	2.09	1	3
1:A:166:ARG:HE	1:A:170:LYS:NZ	0.50	2.05	6	1
1:A:168:HIS:O	1:A:168:HIS:ND1	0.50	2.44	10	4
1:A:132:GLN:O	1:A:133:GLU:CB	0.50	2.60	10	3
1:A:75:ASN:O	1:A:77:PHE:N	0.50	2.44	1	4
1:A:96:ILE:N	1:A:96:ILE:HD12	0.50	2.22	1	4
1:A:143:GLU:O	1:A:144:GLU:C	0.50	2.49	2	2
1:A:75:ASN:N	1:A:75:ASN:HD22	0.50	2.03	1	1
1:A:149:THR:HG22	1:A:150:ALA:H	0.50	1.67	10	2
1:A:88:VAL:HG23	1:A:89:ALA:N	0.50	2.22	9	1
1:A:41:ASP:OD1	1:A:42:ILE:N	0.50	2.45	6	1
1:A:46:ILE:O	1:A:49:ILE:HG22	0.49	2.06	8	1
1:A:132:GLN:C	1:A:134:MET:N	0.49	2.66	3	1
1:A:158:LYS:NZ	1:A:162:GLU:OE2	0.49	2.45	4	2
1:A:35:LEU:N	1:A:35:LEU:CD2	0.49	2.74	5	1
1:A:103:LEU:HD22	1:A:103:LEU:N	0.49	2.22	6	1
1:A:130:GLY:O	1:A:131:ILE:HB	0.49	2.07	3	1
1:A:79:LEU:HD12	1:A:79:LEU:N	0.49	2.22	5	2
1:A:120:PHE:CE2	1:A:124:LYS:NZ	0.49	2.72	10	1
1:A:154:LEU:N	1:A:154:LEU:CD2	0.49	2.75	3	1
1:A:124:LYS:N	1:A:125:PRO:HD2	0.48	2.23	2	5
1:A:131:ILE:O	1:A:132:GLN:CB	0.48	2.60	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:LEU:N	1:A:103:LEU:CD2	0.48	2.76	6	1
1:A:124:LYS:CB	1:A:125:PRO:HD3	0.48	2.39	5	2
1:A:55:LEU:HD12	1:A:55:LEU:N	0.48	2.24	2	3
1:A:79:LEU:O	1:A:171:ASN:ND2	0.48	2.47	10	1
1:A:119:MET:C	1:A:119:MET:SD	0.48	2.92	5	5
1:A:132:GLN:C	1:A:134:MET:H	0.48	2.12	3	1
1:A:136:LYS:O	1:A:140:ASP:N	0.48	2.47	5	2
1:A:130:GLY:O	1:A:131:ILE:O	0.48	2.30	5	1
1:A:131:ILE:O	1:A:131:ILE:CG2	0.48	2.61	10	1
1:A:142:ALA:O	1:A:143:GLU:O	0.47	2.32	4	2
1:A:96:ILE:N	1:A:96:ILE:CD1	0.47	2.77	5	4
1:A:149:THR:CG2	1:A:150:ALA:N	0.47	2.78	1	3
1:A:82:LYS:NZ	1:A:167:VAL:CG2	0.47	2.77	3	1
1:A:148:THR:O	1:A:148:THR:HG22	0.47	2.10	6	1
1:A:118:LEU:O	1:A:118:LEU:HD23	0.47	2.10	3	3
1:A:154:LEU:HD23	1:A:154:LEU:O	0.47	2.10	2	2
1:A:147:PRO:C	1:A:149:THR:H	0.47	2.13	6	2
1:A:147:PRO:C	1:A:149:THR:N	0.47	2.69	6	1
1:A:88:VAL:HG13	1:A:89:ALA:N	0.46	2.26	7	2
1:A:167:VAL:HG23	1:A:168:HIS:N	0.46	2.25	1	1
1:A:75:ASN:C	1:A:77:PHE:N	0.46	2.69	1	2
1:A:118:LEU:HD22	1:A:118:LEU:N	0.46	2.24	4	1
1:A:156:ILE:N	1:A:156:ILE:CD1	0.46	2.78	3	3
1:A:111:GLU:N	1:A:111:GLU:OE1	0.46	2.47	5	1
1:A:132:GLN:OE1	1:A:132:GLN:N	0.46	2.48	6	1
1:A:137:THR:HG23	1:A:138:VAL:N	0.46	2.26	4	1
1:A:175:LEU:HD12	1:A:175:LEU:N	0.46	2.26	7	1
1:A:33:ILE:N	1:A:33:ILE:CD1	0.45	2.79	6	1
1:A:79:LEU:N	1:A:79:LEU:CD1	0.45	2.79	5	3
1:A:75:ASN:N	1:A:75:ASN:OD1	0.45	2.48	7	1
1:A:90:GLU:CG	1:A:91:LYS:N	0.45	2.79	7	2
1:A:124:LYS:CB	1:A:125:PRO:CD	0.45	2.95	3	4
1:A:145:ASN:HD21	1:A:156:ILE:CD1	0.45	2.24	9	1
1:A:132:GLN:O	1:A:133:GLU:HB2	0.45	2.12	8	2
1:A:126:LEU:N	1:A:126:LEU:CD2	0.44	2.80	1	1
1:A:55:LEU:H	1:A:55:LEU:CD2	0.44	2.25	3	1
1:A:119:MET:SD	1:A:119:MET:O	0.44	2.76	5	2
1:A:169:THR:O	1:A:173:CYS:SG	0.44	2.75	7	1
1:A:118:LEU:N	1:A:118:LEU:CD2	0.44	2.80	4	1
1:A:153:VAL:O	1:A:156:ILE:N	0.44	2.50	9	1
1:A:144:GLU:O	1:A:145:ASN:ND2	0.44	2.51	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LEU:HD22	1:A:129:LEU:N	0.44	2.28	10	1
1:A:129:LEU:O	1:A:129:LEU:HD23	0.44	2.11	1	1
1:A:112:PHE:O	1:A:115:MET:N	0.44	2.50	8	1
1:A:158:LYS:O	1:A:162:GLU:CB	0.44	2.66	8	1
1:A:126:LEU:N	1:A:126:LEU:HD22	0.43	2.27	1	1
1:A:145:ASN:O	1:A:145:ASN:ND2	0.43	2.51	3	1
1:A:127:GLN:C	1:A:129:LEU:N	0.43	2.71	3	1
1:A:132:GLN:O	1:A:133:GLU:HG2	0.43	2.13	5	1
1:A:118:LEU:HD13	1:A:118:LEU:O	0.43	2.13	8	2
1:A:131:ILE:HG21	1:A:134:MET:HG3	0.43	1.90	4	1
1:A:137:THR:CG2	1:A:138:VAL:N	0.43	2.81	4	1
1:A:55:LEU:N	1:A:55:LEU:CD1	0.43	2.81	1	3
1:A:168:HIS:C	1:A:168:HIS:ND1	0.43	2.72	3	1
1:A:146:PRO:C	1:A:148:THR:N	0.43	2.71	6	1
1:A:145:ASN:ND2	1:A:156:ILE:CD1	0.43	2.81	9	1
1:A:131:ILE:CG2	1:A:132:GLN:N	0.43	2.75	9	1
1:A:111:GLU:H	1:A:111:GLU:CD	0.43	2.18	9	1
1:A:134:MET:O	1:A:138:VAL:HG12	0.42	2.13	10	1
1:A:138:VAL:CG1	1:A:139:SER:N	0.42	2.82	1	2
1:A:118:LEU:HD12	1:A:118:LEU:N	0.42	2.29	10	1
1:A:130:GLY:O	1:A:131:ILE:CB	0.42	2.67	3	1
1:A:132:GLN:N	1:A:132:GLN:CD	0.42	2.72	6	1
1:A:132:GLN:O	1:A:133:GLU:CG	0.42	2.68	10	2
1:A:129:LEU:N	1:A:129:LEU:CD2	0.42	2.82	10	1
1:A:138:VAL:HG13	1:A:139:SER:N	0.42	2.30	1	3
1:A:170:LYS:O	1:A:174:THR:HG23	0.42	2.14	1	1
1:A:130:GLY:C	1:A:132:GLN:NE2	0.42	2.73	6	1
1:A:149:THR:HG23	1:A:152:GLY:H	0.42	1.75	8	1
1:A:137:THR:CG2	1:A:159:LYS:NZ	0.42	2.82	10	1
1:A:49:ILE:CG2	1:A:50:LYS:N	0.42	2.83	8	1
1:A:145:ASN:ND2	1:A:145:ASN:O	0.42	2.52	9	1
1:A:80:GLU:O	1:A:84:ARG:NH1	0.42	2.53	5	1
1:A:129:LEU:HD23	1:A:129:LEU:O	0.42	2.15	5	1
1:A:127:GLN:C	1:A:129:LEU:H	0.41	2.18	3	1
1:A:48:ALA:O	1:A:52:ASP:OD2	0.41	2.38	5	1
1:A:143:GLU:OE1	1:A:143:GLU:N	0.41	2.49	1	1
1:A:41:ASP:OD1	1:A:41:ASP:N	0.41	2.49	3	1
1:A:143:GLU:N	1:A:143:GLU:CD	0.41	2.74	1	1
1:A:153:VAL:C	1:A:155:GLU:N	0.41	2.74	9	1
1:A:103:LEU:O	1:A:103:LEU:HD13	0.41	2.14	5	1
1:A:147:PRO:O	1:A:149:THR:N	0.41	2.53	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:MET:O	1:A:164:LEU:CB	0.41	2.69	1	1
1:A:121:GLU:O	1:A:125:PRO:CD	0.41	2.69	5	1
1:A:111:GLU:CD	1:A:111:GLU:N	0.41	2.74	9	1
1:A:127:GLN:CG	1:A:128:LYS:N	0.40	2.84	2	1
1:A:153:VAL:O	1:A:155:GLU:N	0.40	2.54	9	1
1:A:168:HIS:ND1	1:A:168:HIS:O	0.40	2.54	5	1
1:A:175:LEU:N	1:A:175:LEU:CD1	0.40	2.84	7	1
1:A:167:VAL:CG2	1:A:168:HIS:N	0.40	2.84	1	1
1:A:131:ILE:O	1:A:132:GLN:CG	0.40	2.70	1	1
1:A:149:THR:OG1	1:A:150:ALA:N	0.40	2.54	5	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/168 (74%)	115±2 (92±1%)	5±2 (4±2%)	5±2 (4±2%)	4	32
All	All	1250/1680 (74%)	1151 (92%)	53 (4%)	46 (4%)	4	32

All 14 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	131	ILE	7
1	A	147	PRO	6
1	A	133	GLU	5
1	A	144	GLU	5
1	A	75	ASN	4
1	A	146	PRO	4
1	A	76	PRO	3
1	A	109	SER	3
1	A	143	GLU	2
1	A	132	GLN	2
1	A	30	ALA	2
1	A	55	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	129	LEU	1
1	A	148	THR	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/142 (75%)	104±2 (97±1%)	3±2 (3±1%)	43	90
All	All	1070/1420 (75%)	1043 (97%)	27 (3%)	43	90

All 17 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	119	MET	6
1	A	75	ASN	2
1	A	154	LEU	2
1	A	134	MET	2
1	A	160	MET	2
1	A	118	LEU	2
1	A	84	ARG	1
1	A	111	GLU	1
1	A	151	GLN	1
1	A	52	ASP	1
1	A	103	LEU	1
1	A	133	GLU	1
1	A	109	SER	1
1	A	144	GLU	1
1	A	127	GLN	1
1	A	129	LEU	1
1	A	171	ASN	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1725
Number of shifts mapped to atoms	1725
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	165	$-0.45 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	155	$0.31 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	146	$-0.48 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	156	$0.02 \pm 0.22$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1357 atoms were assigned a chemical shift out of a possible 1738. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	604/620 (97%)	244/249 (98%)	241/250 (96%)	119/121 (98%)
Sidechain	728/1052 (69%)	483/682 (71%)	245/331 (74%)	0/39 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	25/66 (38%)	14/32 (44%)	11/32 (34%)	0/2 (0%)
Overall	1357/1738 (78%)	741/963 (77%)	497/613 (81%)	119/162 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1725 atoms were assigned a chemical shift out of a possible 2246. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	790/841 (94%)	323/341 (95%)	311/336 (93%)	156/164 (95%)
Sidechain	896/1309 (68%)	591/843 (70%)	305/416 (73%)	0/50 (0%)
Aromatic	39/96 (41%)	22/47 (47%)	17/47 (36%)	0/2 (0%)
Overall	1725/2246 (77%)	936/1231 (76%)	633/799 (79%)	156/216 (72%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

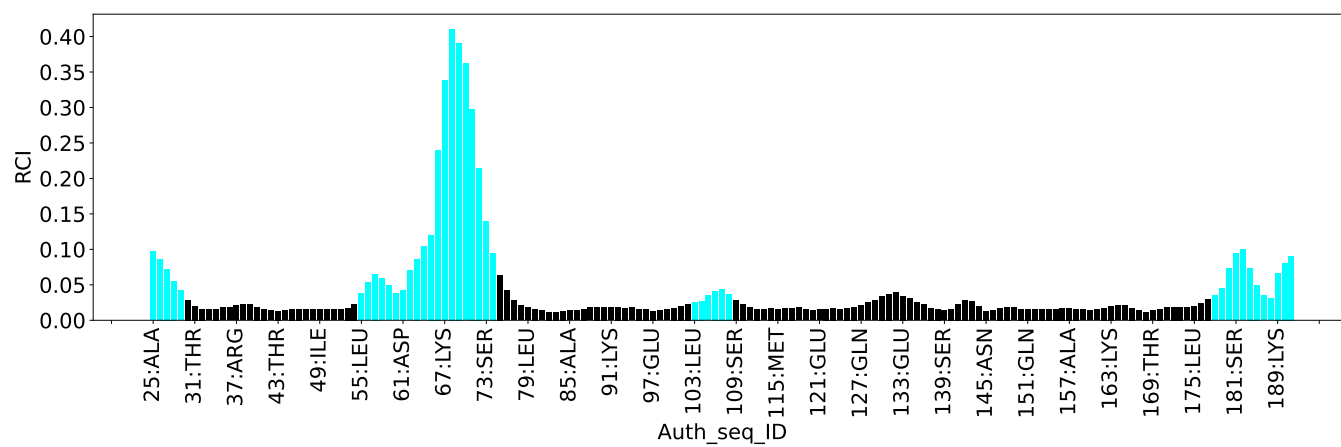
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	145	ASN	C	185.30	166.56 – 184.06	5.7

#### 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	1292
Intra-residue ( $ i-j =0$ )	129
Sequential ( $ i-j =1$ )	269
Medium range ( $ i-j >1$ and $ i-j <5$ )	409
Long range ( $ i-j \geq 5$ )	485
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	210
Number of unmapped restraints	0
Number of restraints per residue	8.9
Number of long range restraints per residue <sup>1</sup>	2.9

<sup>1</sup>Long 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)	23.0	0.2
0.2-0.5 (Medium)	25.1	0.5
>0.5 (Large)	None	None

### 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)	19.8	9.76
10.0-20.0 (Medium)	0.2	10.85
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

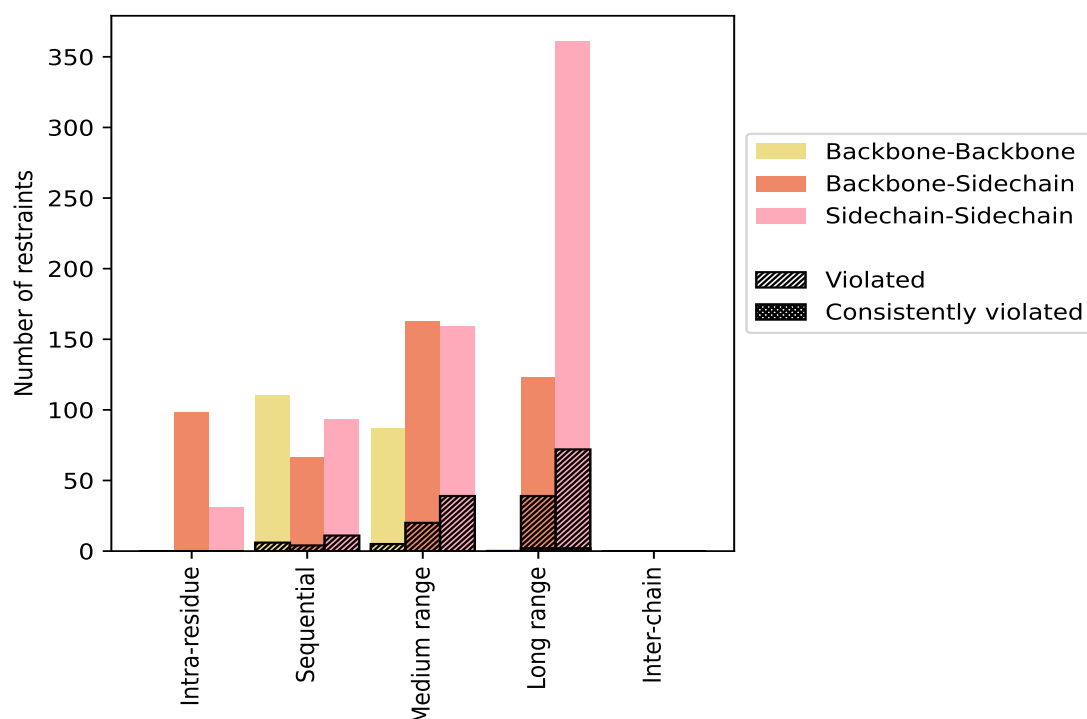
### 9.1 Summary of distance violations ⓘ

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>129</b>	<b>10.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	98	7.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	31	2.4	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>269</b>	<b>20.8</b>	<b>21</b>	<b>7.8</b>	<b>1.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	110	8.5	6	5.5	0.5	0	0.0	0.0
Backbone-Sidechain	66	5.1	4	6.1	0.3	0	0.0	0.0
Sidechain-Sidechain	93	7.2	11	11.8	0.9	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>409</b>	<b>31.7</b>	<b>64</b>	<b>15.6</b>	<b>5.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	87	6.7	5	5.7	0.4	0	0.0	0.0
Backbone-Sidechain	163	12.6	20	12.3	1.5	0	0.0	0.0
Sidechain-Sidechain	159	12.3	39	24.5	3.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>485</b>	<b>37.5</b>	<b>111</b>	<b>22.9</b>	<b>8.6</b>	<b>4</b>	<b>0.8</b>	<b>0.3</b>
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	123	9.5	39	31.7	3.0	2	1.6	0.2
Sidechain-Sidechain	361	27.9	72	19.9	5.6	2	0.6	0.2
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1292</b>	<b>100.0</b>	<b>196</b>	<b>15.2</b>	<b>15.2</b>	<b>4</b>	<b>0.3</b>	<b>0.3</b>
Backbone-Backbone	198	15.3	11	5.6	0.9	0	0.0	0.0
Backbone-Sidechain	450	34.8	63	14.0	4.9	2	0.4	0.2
Sidechain-Sidechain	644	49.8	122	18.9	9.4	2	0.3	0.2

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

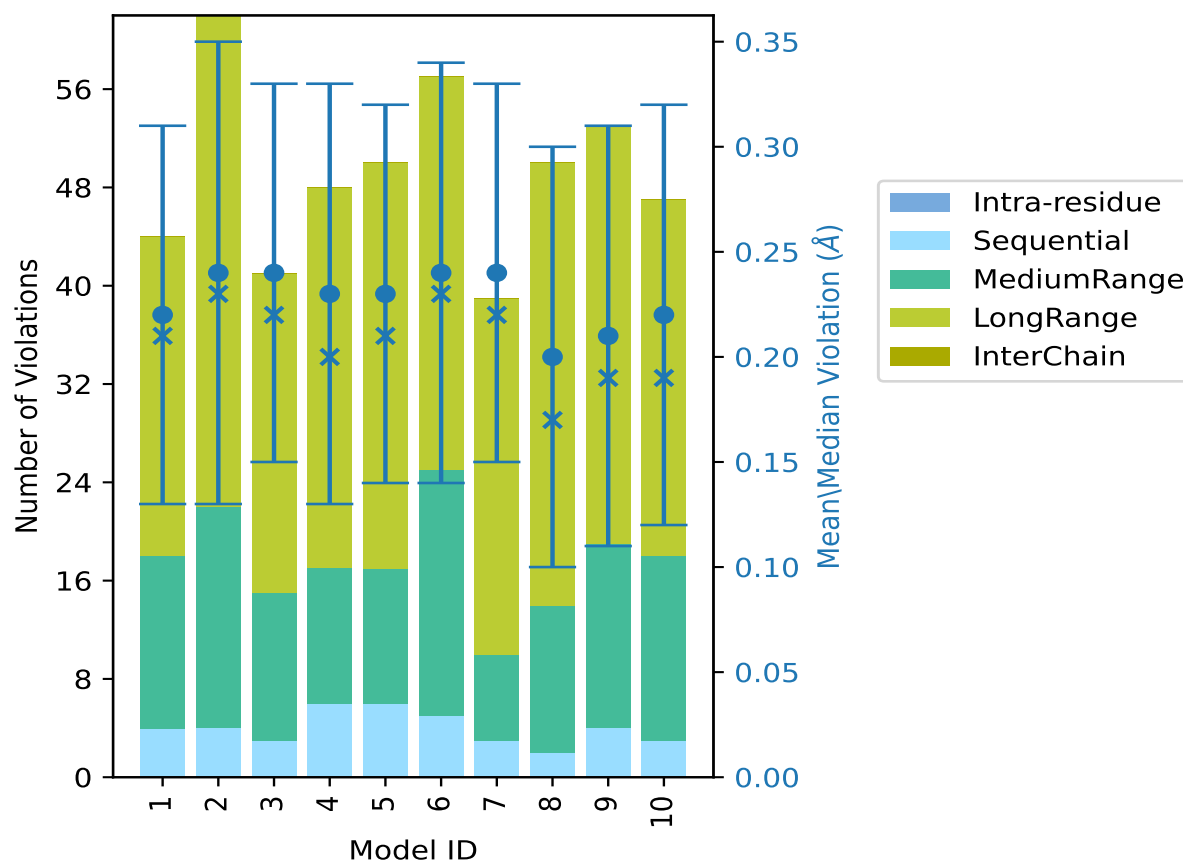
## 9.2 Distance violation statistics for each model [i](#)

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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	4	14	26	0	44	0.22	0.44	0.09	0.21
2	0	4	18	40	0	62	0.24	0.5	0.11	0.23
3	0	3	12	26	0	41	0.24	0.49	0.09	0.22
4	0	6	11	31	0	48	0.23	0.48	0.1	0.2
5	0	6	11	33	0	50	0.23	0.47	0.09	0.21
6	0	5	20	32	0	57	0.24	0.48	0.1	0.23
7	0	3	7	29	0	39	0.24	0.46	0.09	0.22
8	0	2	12	36	0	50	0.2	0.48	0.1	0.17
9	0	4	15	34	0	53	0.21	0.5	0.1	0.19
10	0	3	15	29	0	47	0.22	0.44	0.1	0.19

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard 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, 1096(IR:129, SQ:248, MR:345, LR:374, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	11	29	52	0	92	1	10.0
0	6	19	19	0	44	2	20.0
0	1	8	10	0	19	3	30.0

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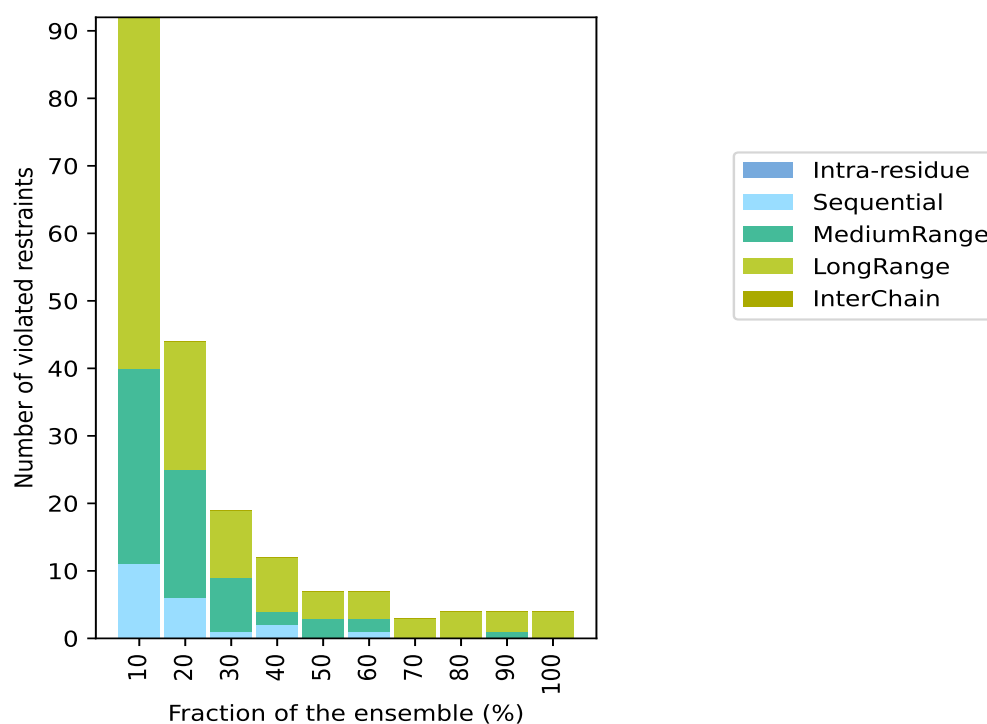
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	2	2	8	0	12	4	40.0
0	0	3	4	0	7	5	50.0
0	1	2	4	0	7	6	60.0
0	0	0	3	0	3	7	70.0
0	0	0	4	0	4	8	80.0
0	0	1	3	0	4	9	90.0
0	0	0	4	0	4	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

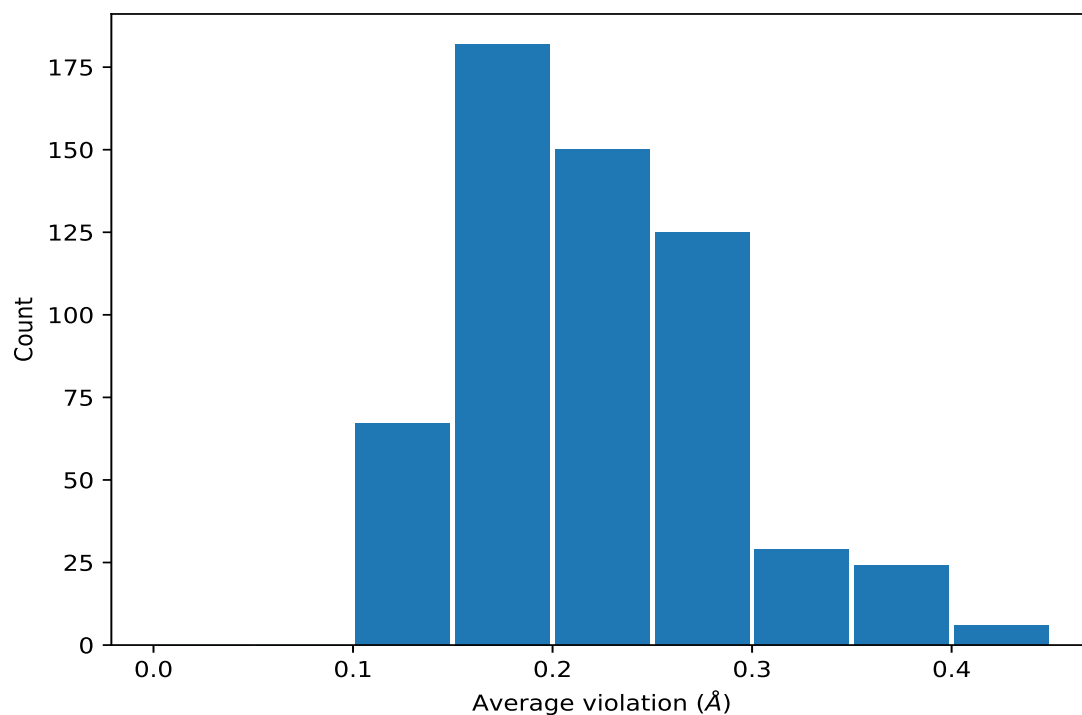


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	10	0.38	0.06	0.38
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	10	0.38	0.06	0.38
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	10	0.38	0.06	0.38
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	10	0.34	0.05	0.32
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	10	0.34	0.05	0.32
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	10	0.34	0.05	0.32
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	10	0.3	0.1	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	10	0.3	0.1	0.29
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	10	0.3	0.1	0.29
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	10	0.24	0.08	0.24
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	10	0.24	0.08	0.24
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	10	0.24	0.08	0.24
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	9	0.33	0.13	0.33
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	9	0.33	0.13	0.33
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	9	0.33	0.13	0.33
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	9	0.33	0.13	0.33
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	9	0.33	0.13	0.33
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	9	0.33	0.13	0.33
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	9	0.3	0.09	0.32
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	9	0.3	0.09	0.32
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	9	0.3	0.09	0.32
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	9	0.21	0.07	0.2
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	9	0.21	0.07	0.2
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	9	0.21	0.07	0.2
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	9	0.21	0.06	0.21
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	9	0.21	0.06	0.21
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	9	0.21	0.06	0.21
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	8	0.29	0.12	0.28
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	8	0.29	0.12	0.28
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	8	0.29	0.12	0.28
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	8	0.25	0.12	0.22
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	8	0.25	0.12	0.22
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	8	0.24	0.07	0.22
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	8	0.24	0.07	0.22
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	8	0.24	0.07	0.22
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	8	0.24	0.07	0.22
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	8	0.24	0.07	0.22
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	8	0.24	0.07	0.22
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	8	0.22	0.08	0.2
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	8	0.22	0.08	0.2
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	8	0.22	0.08	0.2
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	8	0.22	0.08	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	7	0.25	0.04	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	7	0.25	0.04	0.24
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	7	0.24	0.1	0.22
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	7	0.24	0.1	0.22
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	7	0.21	0.07	0.21
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	7	0.21	0.07	0.21
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	7	0.21	0.07	0.21
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	7	0.21	0.07	0.21
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	7	0.21	0.07	0.21
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	7	0.21	0.07	0.21
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG2	6	0.27	0.06	0.28
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG3	6	0.27	0.06	0.28
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB1	6	0.26	0.09	0.28
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB2	6	0.26	0.09	0.28
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB3	6	0.26	0.09	0.28
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB1	6	0.26	0.09	0.28
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB2	6	0.26	0.09	0.28
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB3	6	0.26	0.09	0.28
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB1	6	0.26	0.09	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB2	6	0.26	0.09	0.28
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB3	6	0.26	0.09	0.28
(1,295)	1:137:A:THR:HG21	1:160:A:MET:HA	6	0.23	0.08	0.22
(1,295)	1:137:A:THR:HG22	1:160:A:MET:HA	6	0.23	0.08	0.22
(1,295)	1:137:A:THR:HG23	1:160:A:MET:HA	6	0.23	0.08	0.22
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG21	6	0.23	0.09	0.2
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG22	6	0.23	0.09	0.2
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG23	6	0.23	0.09	0.2
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB1	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB2	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB3	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB1	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB2	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB3	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB1	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB2	6	0.2	0.09	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB3	6	0.2	0.09	0.16
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE1	6	0.18	0.05	0.18
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE2	6	0.18	0.05	0.18
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE3	6	0.18	0.05	0.18
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB2	6	0.15	0.02	0.15
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB3	6	0.15	0.02	0.15
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB2	6	0.15	0.02	0.15
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB3	6	0.15	0.02	0.15
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB2	6	0.15	0.02	0.15
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB3	6	0.15	0.02	0.15
(1,32)	1:104:A:LYS:H	1:107:A:GLY:H	5	0.38	0.1	0.44
(1,475)	1:178:A:LYS:HB2	1:181:A:SER:HA	5	0.33	0.11	0.26
(1,475)	1:178:A:LYS:HB3	1:181:A:SER:HA	5	0.33	0.11	0.26
(1,366)	1:142:A:ALA:HB1	1:146:A:PRO:HD2	5	0.3	0.05	0.31
(1,366)	1:142:A:ALA:HB2	1:146:A:PRO:HD2	5	0.3	0.05	0.31
(1,366)	1:142:A:ALA:HB3	1:146:A:PRO:HD2	5	0.3	0.05	0.31
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB1	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB2	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB3	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB1	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB2	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB3	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB1	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB2	5	0.19	0.05	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB3	5	0.19	0.05	0.22
(1,226)	1:86:A:THR:HG21	1:165:A:GLN:HA	5	0.19	0.08	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,226)	1:86:A:THR:HG22	1:165:A:GLN:HA	5	0.19	0.08	0.14
(1,226)	1:86:A:THR:HG23	1:165:A:GLN:HA	5	0.19	0.08	0.14
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE1	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE2	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE3	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE1	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE2	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE3	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE1	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE2	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE3	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE1	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE2	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE3	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE1	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE2	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE3	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE1	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE2	5	0.18	0.04	0.17
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE3	5	0.18	0.04	0.17
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB1	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB2	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB3	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB1	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB2	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB3	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB1	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB2	5	0.18	0.06	0.17
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB3	5	0.18	0.06	0.17
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG2	4	0.3	0.12	0.29
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG3	4	0.3	0.12	0.29
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG2	4	0.3	0.12	0.29
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG3	4	0.3	0.12	0.29
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD2	4	0.24	0.07	0.26
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD3	4	0.24	0.07	0.26
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD2	4	0.24	0.07	0.26
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD3	4	0.24	0.07	0.26
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD11	4	0.24	0.09	0.24
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD12	4	0.24	0.09	0.24
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD13	4	0.24	0.09	0.24
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD21	4	0.24	0.09	0.24
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD22	4	0.24	0.09	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD23	4	0.24	0.09	0.24
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE1	4	0.24	0.09	0.24
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE2	4	0.24	0.09	0.24
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE3	4	0.24	0.09	0.24
(1,757)	1:183:A:PHE:HE1	1:185:A:ASP:HB3	4	0.23	0.07	0.22
(1,757)	1:183:A:PHE:HE2	1:185:A:ASP:HB3	4	0.23	0.07	0.22
(1,457)	1:147:A:PRO:HG2	1:156:A:ILE:HA	4	0.21	0.04	0.22
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	4	0.19	0.09	0.16
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	4	0.19	0.09	0.16
(1,433)	1:115:A:MET:HE1	1:118:A:LEU:HB2	4	0.17	0.04	0.17
(1,433)	1:115:A:MET:HE2	1:118:A:LEU:HB2	4	0.17	0.04	0.17
(1,433)	1:115:A:MET:HE3	1:118:A:LEU:HB2	4	0.17	0.04	0.17
(1,299)	1:141:A:ALA:HB1	1:155:A:GLU:HA	4	0.16	0.02	0.15
(1,299)	1:141:A:ALA:HB2	1:155:A:GLU:HA	4	0.16	0.02	0.15
(1,299)	1:141:A:ALA:HB3	1:155:A:GLU:HA	4	0.16	0.02	0.15
(1,833)	1:53:A:ALA:HB1	1:60:A:PHE:HZ	4	0.15	0.02	0.14
(1,833)	1:53:A:ALA:HB2	1:60:A:PHE:HZ	4	0.15	0.02	0.14
(1,833)	1:53:A:ALA:HB3	1:60:A:PHE:HZ	4	0.15	0.02	0.14
(1,313)	1:42:A:ILE:HG21	1:126:A:LEU:HA	4	0.15	0.02	0.16
(1,313)	1:42:A:ILE:HG22	1:126:A:LEU:HA	4	0.15	0.02	0.16
(1,313)	1:42:A:ILE:HG23	1:126:A:LEU:HA	4	0.15	0.02	0.16
(1,1059)	1:83:A:VAL:HG11	1:169:A:THR:HA	4	0.12	0.02	0.12
(1,1059)	1:83:A:VAL:HG12	1:169:A:THR:HA	4	0.12	0.02	0.12
(1,1059)	1:83:A:VAL:HG13	1:169:A:THR:HA	4	0.12	0.02	0.12
(1,1059)	1:83:A:VAL:HG21	1:169:A:THR:HA	4	0.12	0.02	0.12
(1,1059)	1:83:A:VAL:HG22	1:169:A:THR:HA	4	0.12	0.02	0.12
(1,1059)	1:83:A:VAL:HG23	1:169:A:THR:HA	4	0.12	0.02	0.12
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD11	3	0.36	0.12	0.44
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD12	3	0.36	0.12	0.44
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD13	3	0.36	0.12	0.44
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD21	3	0.32	0.03	0.33
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD22	3	0.32	0.03	0.33
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD23	3	0.32	0.03	0.33
(1,888)	1:27:A:LEU:HD11	1:32:A:LYS:HA	3	0.26	0.04	0.27
(1,888)	1:27:A:LEU:HD12	1:32:A:LYS:HA	3	0.26	0.04	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,888)	1:27:A:LEU:HD13	1:32:A:LYS:HA	3	0.26	0.04	0.27
(1,888)	1:27:A:LEU:HD21	1:32:A:LYS:HA	3	0.26	0.04	0.27
(1,888)	1:27:A:LEU:HD22	1:32:A:LYS:HA	3	0.26	0.04	0.27
(1,888)	1:27:A:LEU:HD23	1:32:A:LYS:HA	3	0.26	0.04	0.27
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD11	3	0.25	0.08	0.23
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD12	3	0.25	0.08	0.23
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD13	3	0.25	0.08	0.23
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE1	3	0.24	0.06	0.21
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE2	3	0.24	0.06	0.21
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE3	3	0.24	0.06	0.21
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD11	3	0.23	0.04	0.26
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD12	3	0.23	0.04	0.26
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD13	3	0.23	0.04	0.26
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD11	3	0.23	0.04	0.26
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD12	3	0.23	0.04	0.26
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD13	3	0.23	0.04	0.26
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB1	3	0.23	0.08	0.27
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB2	3	0.23	0.08	0.27
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB3	3	0.23	0.08	0.27
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG21	3	0.23	0.06	0.22
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG22	3	0.23	0.06	0.22
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG23	3	0.23	0.06	0.22
(1,322)	1:96:A:ILE:HD11	1:115:A:MET:HA	3	0.21	0.07	0.25
(1,322)	1:96:A:ILE:HD12	1:115:A:MET:HA	3	0.21	0.07	0.25
(1,322)	1:96:A:ILE:HD13	1:115:A:MET:HA	3	0.21	0.07	0.25
(1,558)	1:100:A:ALA:HB1	1:103:A:LEU:HG	3	0.21	0.05	0.18
(1,558)	1:100:A:ALA:HB2	1:103:A:LEU:HG	3	0.21	0.05	0.18
(1,558)	1:100:A:ALA:HB3	1:103:A:LEU:HG	3	0.21	0.05	0.18
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD11	3	0.21	0.01	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD12	3	0.21	0.01	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD13	3	0.21	0.01	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD21	3	0.21	0.01	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD22	3	0.21	0.01	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD23	3	0.21	0.01	0.21
(1,540)	1:101:A:THR:HG21	1:154:A:LEU:HG	3	0.19	0.04	0.22
(1,540)	1:101:A:THR:HG22	1:154:A:LEU:HG	3	0.19	0.04	0.22
(1,540)	1:101:A:THR:HG23	1:154:A:LEU:HG	3	0.19	0.04	0.22
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB2	3	0.18	0.09	0.13
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB3	3	0.18	0.09	0.13
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB2	3	0.18	0.09	0.13
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB3	3	0.18	0.09	0.13
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB2	3	0.18	0.07	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB3	3	0.18	0.07	0.13
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB2	3	0.18	0.07	0.13
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB3	3	0.18	0.07	0.13
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB2	3	0.18	0.07	0.13
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB3	3	0.18	0.07	0.13
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE1	3	0.16	0.04	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE2	3	0.16	0.04	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE3	3	0.16	0.04	0.19
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB2	3	0.16	0.04	0.17
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB3	3	0.16	0.04	0.17
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB2	3	0.16	0.04	0.17
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB3	3	0.16	0.04	0.17
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB2	3	0.16	0.04	0.17
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB3	3	0.16	0.04	0.17
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG21	3	0.14	0.02	0.15
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG22	3	0.14	0.02	0.15
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG23	3	0.14	0.02	0.15
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG21	3	0.14	0.02	0.15
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG22	3	0.14	0.02	0.15
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG23	3	0.14	0.02	0.15
(1,595)	1:82:A:LYS:HG2	1:131:A:ILE:HA	3	0.13	0.03	0.11
(1,595)	1:82:A:LYS:HG3	1:131:A:ILE:HA	3	0.13	0.03	0.11
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD11	3	0.12	0.01	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD12	3	0.12	0.01	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD13	3	0.12	0.01	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD21	3	0.12	0.01	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD22	3	0.12	0.01	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD23	3	0.12	0.01	0.12
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG21	2	0.4	0.02	0.4
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG22	2	0.4	0.02	0.4
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG23	2	0.4	0.02	0.4
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG21	2	0.4	0.02	0.4
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG22	2	0.4	0.02	0.4
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG23	2	0.4	0.02	0.4
(1,172)	1:142:A:ALA:H	1:144:A:GLU:H	2	0.38	0.09	0.38
(1,1289)	1:177:A:LYS:HG2	1:178:A:LYS:HE2	2	0.38	0.08	0.38
(1,1289)	1:177:A:LYS:HG2	1:178:A:LYS:HE3	2	0.38	0.08	0.38
(1,1289)	1:177:A:LYS:HG3	1:178:A:LYS:HE2	2	0.38	0.08	0.38
(1,1289)	1:177:A:LYS:HG3	1:178:A:LYS:HE3	2	0.38	0.08	0.38
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD11	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD12	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD13	2	0.36	0.04	0.36

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD21	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD22	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD23	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD11	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD12	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD13	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD21	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD22	2	0.36	0.04	0.36
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD23	2	0.36	0.04	0.36
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD11	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD12	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD13	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD11	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD12	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD13	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD11	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD12	2	0.33	0.17	0.33
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD13	2	0.33	0.17	0.33
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD11	2	0.32	0.12	0.32
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD12	2	0.32	0.12	0.32
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD13	2	0.32	0.12	0.32
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD21	2	0.32	0.12	0.32
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD22	2	0.32	0.12	0.32
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD23	2	0.32	0.12	0.32
(1,1214)	1:133:A:GLU:HB2	1:136:A:LYS:HE2	2	0.3	0.04	0.3
(1,1214)	1:133:A:GLU:HB2	1:136:A:LYS:HE3	2	0.3	0.04	0.3
(1,1214)	1:133:A:GLU:HB3	1:136:A:LYS:HE2	2	0.3	0.04	0.3
(1,1214)	1:133:A:GLU:HB3	1:136:A:LYS:HE3	2	0.3	0.04	0.3
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD11	2	0.29	0.05	0.29
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD12	2	0.29	0.05	0.29
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD13	2	0.29	0.05	0.29
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD11	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD12	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD13	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD11	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD12	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD13	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD11	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD12	2	0.28	0.09	0.28
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD13	2	0.28	0.09	0.28
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG11	2	0.28	0.04	0.28
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG12	2	0.28	0.04	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG13	2	0.28	0.04	0.28
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG21	2	0.28	0.04	0.28
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG22	2	0.28	0.04	0.28
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG23	2	0.28	0.04	0.28
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG21	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG22	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG23	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG21	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG22	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG23	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG21	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG22	2	0.27	0.04	0.27
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG23	2	0.27	0.04	0.27
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB1	2	0.26	0.14	0.26
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB2	2	0.26	0.14	0.26
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB3	2	0.26	0.14	0.26
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB1	2	0.26	0.14	0.26
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB2	2	0.26	0.14	0.26
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB3	2	0.26	0.14	0.26
(1,1290)	1:178:A:LYS:HB2	1:181:A:SER:HB2	2	0.26	0.04	0.26
(1,1290)	1:178:A:LYS:HB2	1:181:A:SER:HB3	2	0.26	0.04	0.26
(1,1290)	1:178:A:LYS:HB3	1:181:A:SER:HB2	2	0.26	0.04	0.26
(1,1290)	1:178:A:LYS:HB3	1:181:A:SER:HB3	2	0.26	0.04	0.26
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG11	2	0.26	0.02	0.26
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG12	2	0.26	0.02	0.26
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG13	2	0.26	0.02	0.26
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	2	0.26	0.1	0.26
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	2	0.26	0.1	0.26
(1,612)	1:121:A:GLU:HA	1:124:A:LYS:HG3	2	0.25	0.13	0.25
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD11	2	0.24	0.08	0.24
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD12	2	0.24	0.08	0.24
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD13	2	0.24	0.08	0.24
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG11	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG12	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG13	2	0.24	0.1	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG21	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG22	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG23	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG11	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG12	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG13	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG21	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG22	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG23	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG11	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG12	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG13	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG21	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG22	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG23	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG11	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG12	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG13	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG21	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG22	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG23	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG11	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG12	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG13	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG21	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG22	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG23	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG11	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG12	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG13	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG21	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG22	2	0.24	0.1	0.24
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG23	2	0.24	0.1	0.24
(1,56)	1:133:A:GLU:H	1:134:A:MET:H	2	0.24	0.05	0.24
(1,614)	1:28:A:THR:HG21	1:32:A:LYS:HA	2	0.22	0.03	0.22
(1,614)	1:28:A:THR:HG22	1:32:A:LYS:HA	2	0.22	0.03	0.22
(1,614)	1:28:A:THR:HG23	1:32:A:LYS:HA	2	0.22	0.03	0.22
(1,205)	1:183:A:PHE:HA	1:186:A:GLU:HG2	2	0.22	0.06	0.22
(1,182)	1:105:A:GLU:H	1:106:A:THR:H	2	0.22	0.01	0.22
(1,550)	1:30:A:ALA:HB1	1:33:A:ILE:HB	2	0.21	0.02	0.21
(1,550)	1:30:A:ALA:HB2	1:33:A:ILE:HB	2	0.21	0.02	0.21
(1,550)	1:30:A:ALA:HB3	1:33:A:ILE:HB	2	0.21	0.02	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,649)	1:49:A:ILE:HG21	1:50:A:LYS:HG3	2	0.2	0.01	0.2
(1,649)	1:49:A:ILE:HG22	1:50:A:LYS:HG3	2	0.2	0.01	0.2
(1,649)	1:49:A:ILE:HG23	1:50:A:LYS:HG3	2	0.2	0.01	0.2
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD11	2	0.2	0.09	0.2
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD12	2	0.2	0.09	0.2
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD13	2	0.2	0.09	0.2
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD11	2	0.2	0.09	0.2
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD12	2	0.2	0.09	0.2
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD13	2	0.2	0.09	0.2
(1,270)	1:121:A:GLU:HA	1:124:A:LYS:HG2	2	0.2	0.04	0.2
(1,69)	1:57:A:GLY:H	1:58:A:VAL:H	2	0.19	0.05	0.19
(1,510)	1:103:A:LEU:HB2	1:107:A:GLY:HA3	2	0.19	0.03	0.19
(1,510)	1:103:A:LEU:HB3	1:107:A:GLY:HA3	2	0.19	0.03	0.19
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG21	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG22	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG23	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG21	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG22	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG23	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG21	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG22	2	0.19	0.04	0.19
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG23	2	0.19	0.04	0.19
(1,1263)	1:163:A:LYS:HG2	1:166:A:ARG:HD2	2	0.19	0.06	0.19
(1,1263)	1:163:A:LYS:HG2	1:166:A:ARG:HD3	2	0.19	0.06	0.19
(1,1263)	1:163:A:LYS:HG3	1:166:A:ARG:HD2	2	0.19	0.06	0.19
(1,1263)	1:163:A:LYS:HG3	1:166:A:ARG:HD3	2	0.19	0.06	0.19
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG21	2	0.18	0.04	0.18
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG22	2	0.18	0.04	0.18
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG23	2	0.18	0.04	0.18
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG21	2	0.18	0.04	0.18
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG22	2	0.18	0.04	0.18
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG23	2	0.18	0.04	0.18
(1,907)	1:34:A:ARG:HA	1:37:A:ARG:HG2	2	0.18	0.04	0.18
(1,907)	1:34:A:ARG:HA	1:37:A:ARG:HG3	2	0.18	0.04	0.18
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD11	2	0.18	0.01	0.18
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD12	2	0.18	0.01	0.18
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD13	2	0.18	0.01	0.18
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD11	2	0.18	0.01	0.18
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD12	2	0.18	0.01	0.18
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD13	2	0.18	0.01	0.18
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD11	2	0.18	0.01	0.18
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD12	2	0.18	0.01	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD13	2	0.18	0.01	0.18
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD11	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD12	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD13	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD21	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD22	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD23	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD11	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD12	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD13	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD21	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD22	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD23	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD11	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD12	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD13	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD21	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD22	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD23	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD11	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD12	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD13	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD21	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD22	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD23	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD11	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD12	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD13	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD21	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD22	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD23	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD11	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD12	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD13	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD21	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD22	2	0.18	0.02	0.18
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD23	2	0.18	0.02	0.18
(1,883)	1:26:A:GLY:HA2	1:32:A:LYS:HB2	2	0.18	0.06	0.18
(1,883)	1:26:A:GLY:HA2	1:32:A:LYS:HB3	2	0.18	0.06	0.18
(1,883)	1:26:A:GLY:HA3	1:32:A:LYS:HB2	2	0.18	0.06	0.18
(1,883)	1:26:A:GLY:HA3	1:32:A:LYS:HB3	2	0.18	0.06	0.18
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD11	2	0.16	0.0	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD12	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD13	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD21	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD22	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD23	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD11	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD12	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD13	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD21	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD22	2	0.16	0.0	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD23	2	0.16	0.0	0.16
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG11	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG12	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG13	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG21	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG22	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG23	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG11	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG12	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG13	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG21	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG22	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG23	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG11	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG12	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG13	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG21	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG22	2	0.16	0.05	0.16
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG23	2	0.16	0.05	0.16
(1,1276)	1:172:A:TYR:HB2	1:176:A:LYS:HG2	2	0.15	0.05	0.15
(1,1276)	1:172:A:TYR:HB2	1:176:A:LYS:HG3	2	0.15	0.05	0.15
(1,1276)	1:172:A:TYR:HB3	1:176:A:LYS:HG2	2	0.15	0.05	0.15
(1,1276)	1:172:A:TYR:HB3	1:176:A:LYS:HG3	2	0.15	0.05	0.15
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE1	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE2	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE3	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE1	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE2	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE3	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE1	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE2	2	0.15	0.02	0.15
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE3	2	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG11	2	0.14	0.01	0.14
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG12	2	0.14	0.01	0.14
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG13	2	0.14	0.01	0.14
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG21	2	0.14	0.01	0.14
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG22	2	0.14	0.01	0.14
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG23	2	0.14	0.01	0.14
(1,24)	1:150:A:ALA:H	1:153:A:VAL:H	2	0.14	0.02	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD11	2	0.14	0.01	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD12	2	0.14	0.01	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD13	2	0.14	0.01	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD21	2	0.14	0.01	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD22	2	0.14	0.01	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD23	2	0.14	0.01	0.14
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG21	2	0.12	0.02	0.12
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG22	2	0.12	0.02	0.12
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG23	2	0.12	0.02	0.12
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG21	2	0.11	0.0	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG22	2	0.11	0.0	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG23	2	0.11	0.0	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG21	2	0.11	0.0	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG22	2	0.11	0.0	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG23	2	0.11	0.0	0.11

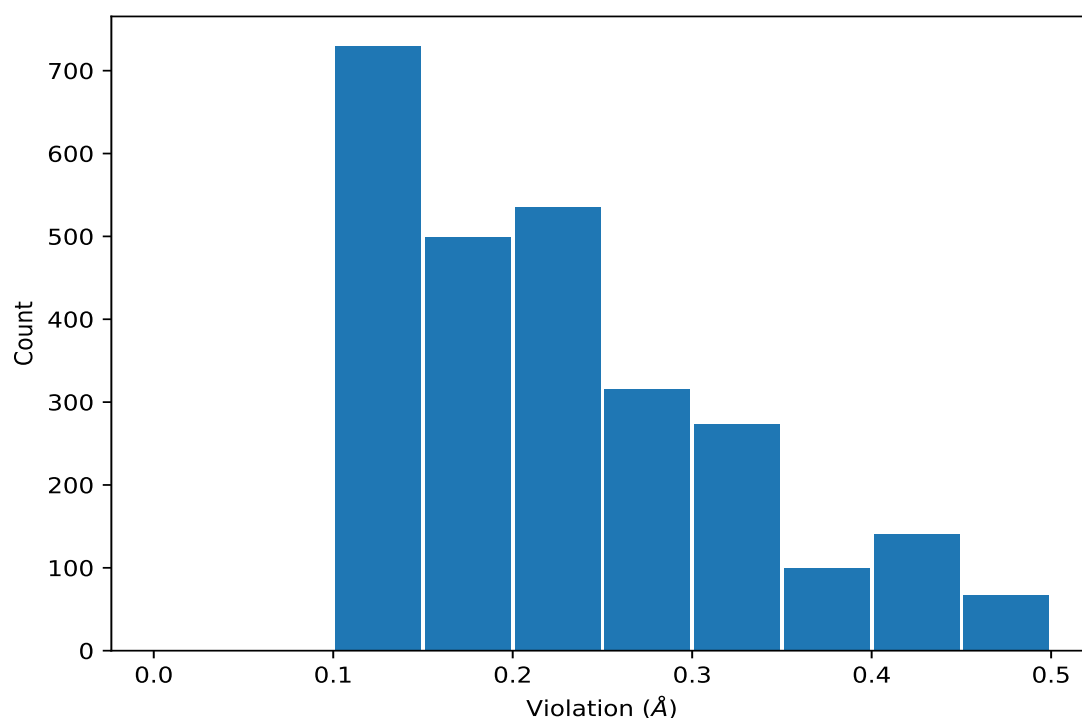
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints ⓘ

### 9.5.1 Histogram : Distribution of distance violations ⓘ

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)
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD11	2	0.5
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD12	2	0.5
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD13	2	0.5
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD11	2	0.5
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD12	2	0.5
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD13	2	0.5
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD11	2	0.5
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD12	2	0.5
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD13	2	0.5
(1,475)	1:178:A:LYS:HB2	1:181:A:SER:HA	9	0.5
(1,475)	1:178:A:LYS:HB3	1:181:A:SER:HA	9	0.5
(1,618)	1:62:A:ALA:HB1	1:78:A:ILE:HG21	2	0.49
(1,618)	1:62:A:ALA:HB1	1:78:A:ILE:HG22	2	0.49
(1,618)	1:62:A:ALA:HB1	1:78:A:ILE:HG23	2	0.49
(1,618)	1:62:A:ALA:HB2	1:78:A:ILE:HG21	2	0.49
(1,618)	1:62:A:ALA:HB2	1:78:A:ILE:HG22	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:62:A:ALA:HB2	1:78:A:ILE:HG23	2	0.49
(1,618)	1:62:A:ALA:HB3	1:78:A:ILE:HG21	2	0.49
(1,618)	1:62:A:ALA:HB3	1:78:A:ILE:HG22	2	0.49
(1,618)	1:62:A:ALA:HB3	1:78:A:ILE:HG23	2	0.49
(1,32)	1:104:A:LYS:H	1:107:A:GLY:H	3	0.49
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	4	0.48
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	4	0.48
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	4	0.48
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	4	0.48
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	4	0.48
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	4	0.48
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	8	0.48
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	8	0.48
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	8	0.48
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	8	0.48
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	8	0.48
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	8	0.48
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	6	0.48
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	6	0.48
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	6	0.48
(1,1138)	1:103:A:LEU:HG	1:104:A:LYS:HB2	5	0.47
(1,1138)	1:103:A:LEU:HG	1:104:A:LYS:HB3	5	0.47
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	9	0.47
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	9	0.47
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	4	0.47
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	4	0.47
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	4	0.47
(1,32)	1:104:A:LYS:H	1:107:A:GLY:H	2	0.47
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	8	0.46
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	8	0.46
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	8	0.46
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	7	0.46
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	7	0.46
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	7	0.46
(1,172)	1:142:A:ALA:H	1:144:A:GLU:H	4	0.46
(1,1289)	1:177:A:LYS:HG2	1:178:A:LYS:HE2	9	0.45
(1,1289)	1:177:A:LYS:HG2	1:178:A:LYS:HE3	9	0.45
(1,1289)	1:177:A:LYS:HG3	1:178:A:LYS:HE2	9	0.45
(1,1289)	1:177:A:LYS:HG3	1:178:A:LYS:HE3	9	0.45
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD11	6	0.45
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD12	6	0.45
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD13	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD21	6	0.45
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD22	6	0.45
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD23	6	0.45
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD11	8	0.45
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD12	8	0.45
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD13	8	0.45
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	5	0.45
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	5	0.45
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	5	0.45
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	10	0.44
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	10	0.44
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	10	0.44
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	10	0.44
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	10	0.44
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	10	0.44
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD11	9	0.44
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD12	9	0.44
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD13	9	0.44
(1,578)	1:30:A:ALA:HA	1:33:A:ILE:HB	1	0.44
(1,32)	1:104:A:LYS:H	1:107:A:GLY:H	6	0.44
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG2	5	0.43
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG3	5	0.43
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG2	5	0.43
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG3	5	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	5	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	5	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	5	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	5	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	5	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	5	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	5	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	5	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	5	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	5	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	5	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	5	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	5	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	5	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	5	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	5	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	5	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	10	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	10	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	10	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	10	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	10	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	10	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	10	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	10	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	10	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	10	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	10	0.43
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	10	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	10	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	10	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	10	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	10	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	10	0.43
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	10	0.43
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	3	0.43
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	3	0.43
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	3	0.43
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	3	0.43
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	3	0.43
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	3	0.43
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	3	0.43
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	3	0.43
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	3	0.43
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	6	0.42
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	6	0.42
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	6	0.42
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	6	0.42
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	6	0.42
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	6	0.42
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	6	0.42
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	6	0.42
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	6	0.42
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	6	0.42
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	6	0.42
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	6	0.42
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	6	0.42
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	6	0.42
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	6	0.42
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	6	0.42
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	6	0.42
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG21	6	0.42
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG22	6	0.42
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG23	6	0.42
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG21	6	0.42
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG22	6	0.42
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG23	6	0.42
(1,845)	1:59:A:ASN:HB3	1:78:A:ILE:HD11	2	0.42
(1,845)	1:59:A:ASN:HB3	1:78:A:ILE:HD12	2	0.42
(1,845)	1:59:A:ASN:HB3	1:78:A:ILE:HD13	2	0.42
(1,475)	1:178:A:LYS:HB2	1:181:A:SER:HA	2	0.42
(1,475)	1:178:A:LYS:HB3	1:181:A:SER:HA	2	0.42
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	2	0.42
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	2	0.42
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	2	0.42
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	5	0.42
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	5	0.42
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	5	0.42
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	7	0.41
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	7	0.41
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	7	0.41
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	7	0.41
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	7	0.41
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	7	0.41
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG21	8	0.41
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG22	8	0.41
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG23	8	0.41
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG2	2	0.4
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG3	2	0.4
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG2	2	0.4
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG3	2	0.4
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD11	1	0.4
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD12	1	0.4
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD13	1	0.4
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD21	1	0.4
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD22	1	0.4
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD23	1	0.4
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD11	1	0.4
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD12	1	0.4
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD13	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD21	1	0.4
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD22	1	0.4
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD23	1	0.4
(1,1112)	1:94:A:ILE:HD11	1:161:A:ARG:HB2	6	0.4
(1,1112)	1:94:A:ILE:HD11	1:161:A:ARG:HB3	6	0.4
(1,1112)	1:94:A:ILE:HD12	1:161:A:ARG:HB2	6	0.4
(1,1112)	1:94:A:ILE:HD12	1:161:A:ARG:HB3	6	0.4
(1,1112)	1:94:A:ILE:HD13	1:161:A:ARG:HB2	6	0.4
(1,1112)	1:94:A:ILE:HD13	1:161:A:ARG:HB3	6	0.4
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB1	6	0.4
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB2	6	0.4
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB3	6	0.4
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB1	6	0.4
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB2	6	0.4
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB3	6	0.4
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	1	0.4
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	1	0.4
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	1	0.4
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	7	0.4
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	7	0.4
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	7	0.4
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	2	0.4
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	2	0.4
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	2	0.4
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	7	0.39
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	7	0.39
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	7	0.39
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	7	0.39
(1,658)	1:131:A:ILE:HG21	1:137:A:THR:HG21	1	0.39
(1,658)	1:131:A:ILE:HG21	1:137:A:THR:HG22	1	0.39
(1,658)	1:131:A:ILE:HG21	1:137:A:THR:HG23	1	0.39
(1,658)	1:131:A:ILE:HG22	1:137:A:THR:HG21	1	0.39
(1,658)	1:131:A:ILE:HG22	1:137:A:THR:HG22	1	0.39
(1,658)	1:131:A:ILE:HG22	1:137:A:THR:HG23	1	0.39
(1,658)	1:131:A:ILE:HG23	1:137:A:THR:HG21	1	0.39
(1,658)	1:131:A:ILE:HG23	1:137:A:THR:HG22	1	0.39
(1,658)	1:131:A:ILE:HG23	1:137:A:THR:HG23	1	0.39
(1,328)	1:90:A:GLU:HA	1:91:A:LYS:HG2	5	0.39
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	10	0.39
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	10	0.39
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	10	0.39
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	1	0.38
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	1	0.38
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	1	0.38
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	1	0.38
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	1	0.38
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	1	0.38
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	1	0.38
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	1	0.38
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	1	0.38
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	1	0.38
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	1	0.38
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	1	0.38
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	1	0.38
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	1	0.38
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	1	0.38
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	1	0.38
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	1	0.38
(1,612)	1:121:A:GLU:HA	1:124:A:LYS:HG3	6	0.38
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB1	9	0.38
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB2	9	0.38
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB3	9	0.38
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB1	9	0.38
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB2	9	0.38
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB3	9	0.38
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB1	9	0.38
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB2	9	0.38
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB3	9	0.38
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	3	0.38
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	3	0.38
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	3	0.38
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG21	10	0.37
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG22	10	0.37
(1,1024)	1:74:A:GLU:HG2	1:78:A:ILE:HG23	10	0.37
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG21	10	0.37
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG22	10	0.37
(1,1024)	1:74:A:GLU:HG3	1:78:A:ILE:HG23	10	0.37
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD11	3	0.37
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD12	3	0.37
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD13	3	0.37
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD11	3	0.37
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD12	3	0.37
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD13	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD11	3	0.37
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD12	3	0.37
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD13	3	0.37
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	5	0.37
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	5	0.37
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	5	0.37
(1,295)	1:137:A:THR:HG21	1:160:A:MET:HA	7	0.37
(1,295)	1:137:A:THR:HG22	1:160:A:MET:HA	7	0.37
(1,295)	1:137:A:THR:HG23	1:160:A:MET:HA	7	0.37
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB1	4	0.36
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB2	4	0.36
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB3	4	0.36
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB1	4	0.36
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB2	4	0.36
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB3	4	0.36
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB1	4	0.36
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB2	4	0.36
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB3	4	0.36
(1,835)	1:46:A:ILE:HG21	1:60:A:PHE:HZ	3	0.36
(1,835)	1:46:A:ILE:HG22	1:60:A:PHE:HZ	3	0.36
(1,835)	1:46:A:ILE:HG23	1:60:A:PHE:HZ	3	0.36
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	7	0.36
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	7	0.36
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	7	0.36
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	7	0.36
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	7	0.36
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	7	0.36
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	7	0.36
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	7	0.36
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	7	0.36
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD11	10	0.36
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD12	10	0.36
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD13	10	0.36
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	3	0.36
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	3	0.36
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	3	0.36
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD21	6	0.36
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD22	6	0.36
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD23	6	0.36
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD11	9	0.35
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD12	9	0.35
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD13	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD21	9	0.35
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD22	9	0.35
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD23	9	0.35
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	2	0.35
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	2	0.35
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	4	0.35
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	4	0.35
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	4	0.35
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	4	0.35
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	4	0.35
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	4	0.35
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	3	0.35
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	3	0.35
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	3	0.35
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE1	2	0.35
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE2	2	0.35
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE3	2	0.35
(1,366)	1:142:A:ALA:HB1	1:146:A:PRO:HD2	2	0.35
(1,366)	1:142:A:ALA:HB2	1:146:A:PRO:HD2	2	0.35
(1,366)	1:142:A:ALA:HB3	1:146:A:PRO:HD2	2	0.35
(1,366)	1:142:A:ALA:HB1	1:146:A:PRO:HD2	4	0.35
(1,366)	1:142:A:ALA:HB2	1:146:A:PRO:HD2	4	0.35
(1,366)	1:142:A:ALA:HB3	1:146:A:PRO:HD2	4	0.35
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG2	7	0.34
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG3	7	0.34
(1,1214)	1:133:A:GLU:HB2	1:136:A:LYS:HE2	2	0.34
(1,1214)	1:133:A:GLU:HB2	1:136:A:LYS:HE3	2	0.34
(1,1214)	1:133:A:GLU:HB3	1:136:A:LYS:HE2	2	0.34
(1,1214)	1:133:A:GLU:HB3	1:136:A:LYS:HE3	2	0.34
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB1	1	0.34
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB2	1	0.34
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB3	1	0.34
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB1	1	0.34
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB2	1	0.34
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB3	1	0.34
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB1	1	0.34
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB2	1	0.34
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB3	1	0.34
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	4	0.34
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	4	0.34
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	4	0.34
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	4	0.34
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	4	0.34
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	8	0.34
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	8	0.34
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	8	0.34
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	8	0.34
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	8	0.34
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	8	0.34
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	1	0.34
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	1	0.34
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	1	0.34
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	4	0.34
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	4	0.34
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	4	0.34
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	4	0.34
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	4	0.34
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	4	0.34
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	9	0.34
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	9	0.34
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	9	0.34
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG11	10	0.33
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG12	10	0.33
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG13	10	0.33
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG21	10	0.33
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG22	10	0.33
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG23	10	0.33
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG11	10	0.33
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG12	10	0.33
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG13	10	0.33
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG21	10	0.33
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG22	10	0.33
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG23	10	0.33
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG11	10	0.33
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG12	10	0.33
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG13	10	0.33
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG21	10	0.33
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG22	10	0.33
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG23	10	0.33
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG11	10	0.33
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG12	10	0.33
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG13	10	0.33
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG21	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG22	10	0.33
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG23	10	0.33
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG11	10	0.33
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG12	10	0.33
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG13	10	0.33
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG21	10	0.33
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG22	10	0.33
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG23	10	0.33
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG11	10	0.33
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG12	10	0.33
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG13	10	0.33
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG21	10	0.33
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG22	10	0.33
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG23	10	0.33
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD11	4	0.33
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD12	4	0.33
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD13	4	0.33
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD21	4	0.33
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD22	4	0.33
(1,1135)	1:102:A:LYS:HE2	1:103:A:LEU:HD23	4	0.33
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD11	4	0.33
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD12	4	0.33
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD13	4	0.33
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD21	4	0.33
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD22	4	0.33
(1,1135)	1:102:A:LYS:HE3	1:103:A:LEU:HD23	4	0.33
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	2	0.33
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	2	0.33
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	2	0.33
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	2	0.33
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	2	0.33
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	2	0.33
(1,911)	1:34:A:ARG:HG2	1:95:A:ALA:HB1	10	0.33
(1,911)	1:34:A:ARG:HG2	1:95:A:ALA:HB2	10	0.33
(1,911)	1:34:A:ARG:HG2	1:95:A:ALA:HB3	10	0.33
(1,911)	1:34:A:ARG:HG3	1:95:A:ALA:HB1	10	0.33
(1,911)	1:34:A:ARG:HG3	1:95:A:ALA:HB2	10	0.33
(1,911)	1:34:A:ARG:HG3	1:95:A:ALA:HB3	10	0.33
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB1	9	0.33
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB2	9	0.33
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB3	9	0.33
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB1	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB2	9	0.33
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB3	9	0.33
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB1	9	0.33
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB2	9	0.33
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB3	9	0.33
(1,757)	1:183:A:PHE:HE1	1:185:A:ASP:HB3	2	0.33
(1,757)	1:183:A:PHE:HE2	1:185:A:ASP:HB3	2	0.33
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD11	6	0.33
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD12	6	0.33
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD13	6	0.33
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	9	0.33
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	9	0.33
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	9	0.33
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	9	0.33
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	9	0.33
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	9	0.33
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	9	0.33
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	9	0.33
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	9	0.33
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	2	0.33
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	2	0.33
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	2	0.33
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	10	0.33
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	10	0.33
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	10	0.33
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	10	0.33
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	10	0.33
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	10	0.33
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD21	2	0.33
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD22	2	0.33
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD23	2	0.33
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG2	10	0.32
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG3	10	0.32
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	7	0.32
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	7	0.32
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	7	0.32
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	7	0.32
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	7	0.32
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	7	0.32
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	7	0.32
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	7	0.32
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	7	0.32
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	7	0.32
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	7	0.32
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	7	0.32
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	7	0.32
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	7	0.32
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	7	0.32
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	7	0.32
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	7	0.32
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	10	0.32
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	10	0.32
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD2	3	0.32
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD3	3	0.32
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD2	3	0.32
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD3	3	0.32
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD11	2	0.32
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD12	2	0.32
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD13	2	0.32
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	5	0.32
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	5	0.32
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	5	0.32
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	10	0.32
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	10	0.32
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	10	0.32
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	2	0.32
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	2	0.32
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	2	0.32
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	3	0.32
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	3	0.32
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	3	0.32
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	9	0.32
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	9	0.32
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	9	0.32
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE1	6	0.32
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE2	6	0.32
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE3	6	0.32
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG11	10	0.31
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG12	10	0.31
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG13	10	0.31
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG21	10	0.31
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG22	10	0.31
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG23	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD11	4	0.31
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD12	4	0.31
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD13	4	0.31
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD21	4	0.31
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD22	4	0.31
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD23	4	0.31
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	5	0.31
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	5	0.31
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	5	0.31
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	5	0.31
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	5	0.31
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	5	0.31
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	4	0.31
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	4	0.31
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	4	0.31
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	4	0.31
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	4	0.31
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	4	0.31
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	4	0.31
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	4	0.31
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	4	0.31
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	4	0.31
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	4	0.31
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	4	0.31
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	4	0.31
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	4	0.31
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	4	0.31
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	4	0.31
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	4	0.31
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	4	0.31
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG21	5	0.31
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG22	5	0.31
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG23	5	0.31
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG21	5	0.31
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG22	5	0.31
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG23	5	0.31
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG21	5	0.31
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG22	5	0.31
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG23	5	0.31
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	9	0.31
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	9	0.31
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	9	0.31
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	9	0.31
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	9	0.31
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	9	0.31
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	9	0.31
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	9	0.31
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB1	9	0.31
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB2	9	0.31
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB3	9	0.31
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE1	4	0.31
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE2	4	0.31
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE3	4	0.31
(1,366)	1:142:A:ALA:HB1	1:146:A:PRO:HD2	6	0.31
(1,366)	1:142:A:ALA:HB2	1:146:A:PRO:HD2	6	0.31
(1,366)	1:142:A:ALA:HB3	1:146:A:PRO:HD2	6	0.31
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	7	0.31
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	7	0.31
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	7	0.31
(1,1290)	1:178:A:LYS:HB2	1:181:A:SER:HB2	8	0.3
(1,1290)	1:178:A:LYS:HB2	1:181:A:SER:HB3	8	0.3
(1,1290)	1:178:A:LYS:HB3	1:181:A:SER:HB2	8	0.3
(1,1290)	1:178:A:LYS:HB3	1:181:A:SER:HB3	8	0.3
(1,1289)	1:177:A:LYS:HG2	1:178:A:LYS:HE2	7	0.3
(1,1289)	1:177:A:LYS:HG2	1:178:A:LYS:HE3	7	0.3
(1,1289)	1:177:A:LYS:HG3	1:178:A:LYS:HE2	7	0.3
(1,1289)	1:177:A:LYS:HG3	1:178:A:LYS:HE3	7	0.3
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	5	0.3
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	5	0.3
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	5	0.3
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	5	0.3
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	10	0.3
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	10	0.3
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	10	0.3
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	10	0.3
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	10	0.3
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	10	0.3
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	10	0.3
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	10	0.3
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	10	0.3
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	10	0.3
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	10	0.3
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	10	0.3
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	10	0.3
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	10	0.3
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	10	0.3
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	10	0.3
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	10	0.3
(1,888)	1:27:A:LEU:HD11	1:32:A:LYS:HA	8	0.3
(1,888)	1:27:A:LEU:HD12	1:32:A:LYS:HA	8	0.3
(1,888)	1:27:A:LEU:HD13	1:32:A:LYS:HA	8	0.3
(1,888)	1:27:A:LEU:HD21	1:32:A:LYS:HA	8	0.3
(1,888)	1:27:A:LEU:HD22	1:32:A:LYS:HA	8	0.3
(1,888)	1:27:A:LEU:HD23	1:32:A:LYS:HA	8	0.3
(1,699)	1:42:A:ILE:HD11	1:88:A:VAL:HB	7	0.3
(1,699)	1:42:A:ILE:HD12	1:88:A:VAL:HB	7	0.3
(1,699)	1:42:A:ILE:HD13	1:88:A:VAL:HB	7	0.3
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	4	0.3
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	4	0.3
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	4	0.3
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB2	10	0.3
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB3	10	0.3
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB2	10	0.3
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB3	10	0.3
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	8	0.3
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	8	0.3
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	8	0.3
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG21	2	0.3
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG22	2	0.3
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG23	2	0.3
(1,226)	1:86:A:THR:HG21	1:165:A:GLN:HA	3	0.3
(1,226)	1:86:A:THR:HG22	1:165:A:GLN:HA	3	0.3
(1,226)	1:86:A:THR:HG23	1:165:A:GLN:HA	3	0.3
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	1	0.29
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	1	0.29
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	1	0.29
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	1	0.29
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	1	0.29
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	1	0.29
(1,690)	1:74:A:GLU:HA	1:79:A:LEU:HD21	8	0.29
(1,690)	1:74:A:GLU:HA	1:79:A:LEU:HD22	8	0.29
(1,690)	1:74:A:GLU:HA	1:79:A:LEU:HD23	8	0.29
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD11	7	0.29
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD12	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD13	7	0.29
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD11	7	0.29
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD12	7	0.29
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD13	7	0.29
(1,558)	1:100:A:ALA:HB1	1:103:A:LEU:HG	1	0.29
(1,558)	1:100:A:ALA:HB2	1:103:A:LEU:HG	1	0.29
(1,558)	1:100:A:ALA:HB3	1:103:A:LEU:HG	1	0.29
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	2	0.29
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	2	0.29
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	2	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	1	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	1	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	1	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	6	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	6	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	6	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB1	7	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB2	7	0.29
(1,293)	1:43:A:THR:HA	1:89:A:ALA:HB3	7	0.29
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	8	0.29
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	8	0.29
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	8	0.29
(1,172)	1:142:A:ALA:H	1:144:A:GLU:H	2	0.29
(1,56)	1:133:A:GLU:H	1:134:A:MET:H	2	0.29
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG2	6	0.28
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG3	6	0.28
(1,1211)	1:132:A:GLN:HG2	1:133:A:GLU:HG2	4	0.28
(1,1211)	1:132:A:GLN:HG2	1:133:A:GLU:HG3	4	0.28
(1,1211)	1:132:A:GLN:HG3	1:133:A:GLU:HG2	4	0.28
(1,1211)	1:132:A:GLN:HG3	1:133:A:GLU:HG3	4	0.28
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD2	4	0.28
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD3	4	0.28
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD2	4	0.28
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD3	4	0.28
(1,895)	1:31:A:THR:HG21	1:33:A:ILE:HG12	6	0.28
(1,895)	1:31:A:THR:HG21	1:33:A:ILE:HG13	6	0.28
(1,895)	1:31:A:THR:HG22	1:33:A:ILE:HG12	6	0.28
(1,895)	1:31:A:THR:HG22	1:33:A:ILE:HG13	6	0.28
(1,895)	1:31:A:THR:HG23	1:33:A:ILE:HG12	6	0.28
(1,895)	1:31:A:THR:HG23	1:33:A:ILE:HG13	6	0.28
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	5	0.28
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	5	0.28
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	5	0.28
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	5	0.28
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	5	0.28
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	5	0.28
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	5	0.28
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	5	0.28
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	6	0.28
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	6	0.28
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	6	0.28
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB1	2	0.28
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB2	2	0.28
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB3	2	0.28
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB1	2	0.28
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB2	2	0.28
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB3	2	0.28
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB1	2	0.28
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB2	2	0.28
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB3	2	0.28
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG21	3	0.28
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG22	3	0.28
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG23	3	0.28
(1,385)	1:101:A:THR:HG21	1:102:A:LYS:HE2	6	0.28
(1,385)	1:101:A:THR:HG21	1:102:A:LYS:HE3	6	0.28
(1,385)	1:101:A:THR:HG22	1:102:A:LYS:HE2	6	0.28
(1,385)	1:101:A:THR:HG22	1:102:A:LYS:HE3	6	0.28
(1,385)	1:101:A:THR:HG23	1:102:A:LYS:HE2	6	0.28
(1,385)	1:101:A:THR:HG23	1:102:A:LYS:HE3	6	0.28
(1,322)	1:96:A:ILE:HD11	1:115:A:MET:HA	10	0.28
(1,322)	1:96:A:ILE:HD12	1:115:A:MET:HA	10	0.28
(1,322)	1:96:A:ILE:HD13	1:115:A:MET:HA	10	0.28
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD21	3	0.28
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD22	3	0.28
(1,276)	1:115:A:MET:HA	1:118:A:LEU:HD23	3	0.28
(1,254)	1:46:A:ILE:HG21	1:87:A:THR:HB	1	0.28
(1,254)	1:46:A:ILE:HG22	1:87:A:THR:HB	1	0.28
(1,254)	1:46:A:ILE:HG23	1:87:A:THR:HB	1	0.28
(1,32)	1:104:A:LYS:H	1:107:A:GLY:H	8	0.28
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG2	8	0.27
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG3	8	0.27
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB2	8	0.27
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB3	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB2	8	0.27
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB3	8	0.27
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB2	8	0.27
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB3	8	0.27
(1,888)	1:27:A:LEU:HD11	1:32:A:LYS:HA	4	0.27
(1,888)	1:27:A:LEU:HD12	1:32:A:LYS:HA	4	0.27
(1,888)	1:27:A:LEU:HD13	1:32:A:LYS:HA	4	0.27
(1,888)	1:27:A:LEU:HD21	1:32:A:LYS:HA	4	0.27
(1,888)	1:27:A:LEU:HD22	1:32:A:LYS:HA	4	0.27
(1,888)	1:27:A:LEU:HD23	1:32:A:LYS:HA	4	0.27
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	1	0.27
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	1	0.27
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	1	0.27
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB1	3	0.27
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB2	3	0.27
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB3	3	0.27
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD11	6	0.27
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD12	6	0.27
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD13	6	0.27
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD11	6	0.27
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD12	6	0.27
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD13	6	0.27
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG11	1	0.27
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG12	1	0.27
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG13	1	0.27
(1,366)	1:142:A:ALA:HB1	1:146:A:PRO:HD2	3	0.27
(1,366)	1:142:A:ALA:HB2	1:146:A:PRO:HD2	3	0.27
(1,366)	1:142:A:ALA:HB3	1:146:A:PRO:HD2	3	0.27
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	6	0.27
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	6	0.27
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	6	0.27
(1,295)	1:137:A:THR:HG21	1:160:A:MET:HA	5	0.27
(1,295)	1:137:A:THR:HG22	1:160:A:MET:HA	5	0.27
(1,295)	1:137:A:THR:HG23	1:160:A:MET:HA	5	0.27
(1,205)	1:183:A:PHE:HA	1:186:A:GLU:HG2	3	0.27
(1,195)	1:101:A:THR:H	1:104:A:LYS:H	6	0.27
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE1	4	0.26
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE2	4	0.26
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE3	4	0.26
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE1	4	0.26
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE2	4	0.26
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE3	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE1	4	0.26
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE2	4	0.26
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE3	4	0.26
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE1	4	0.26
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE2	4	0.26
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE3	4	0.26
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE1	4	0.26
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE2	4	0.26
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE3	4	0.26
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE1	4	0.26
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE2	4	0.26
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE3	4	0.26
(1,1214)	1:133:A:GLU:HB2	1:136:A:LYS:HE2	6	0.26
(1,1214)	1:133:A:GLU:HB2	1:136:A:LYS:HE3	6	0.26
(1,1214)	1:133:A:GLU:HB3	1:136:A:LYS:HE2	6	0.26
(1,1214)	1:133:A:GLU:HB3	1:136:A:LYS:HE3	6	0.26
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	2	0.26
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	2	0.26
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	2	0.26
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	2	0.26
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	2	0.26
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	2	0.26
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	2	0.26
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	2	0.26
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	2	0.26
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	2	0.26
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	2	0.26
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	2	0.26
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	2	0.26
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	2	0.26
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	2	0.26
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	2	0.26
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	2	0.26
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	2	0.26
(1,757)	1:183:A:PHE:HE1	1:185:A:ASP:HB3	5	0.26
(1,757)	1:183:A:PHE:HE2	1:185:A:ASP:HB3	5	0.26
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB1	5	0.26
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB2	5	0.26
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB3	5	0.26
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB1	5	0.26
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB2	5	0.26
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB3	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB1	5	0.26
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB2	5	0.26
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB3	5	0.26
(1,475)	1:178:A:LYS:HB2	1:181:A:SER:HA	7	0.26
(1,475)	1:178:A:LYS:HB3	1:181:A:SER:HA	7	0.26
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD11	3	0.26
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD12	3	0.26
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD13	3	0.26
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD11	3	0.26
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD12	3	0.26
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD13	3	0.26
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	1	0.26
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	1	0.26
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	1	0.26
(1,226)	1:86:A:THR:HG21	1:165:A:GLN:HA	1	0.26
(1,226)	1:86:A:THR:HG22	1:165:A:GLN:HA	1	0.26
(1,226)	1:86:A:THR:HG23	1:165:A:GLN:HA	1	0.26
(1,1263)	1:163:A:LYS:HG2	1:166:A:ARG:HD2	9	0.25
(1,1263)	1:163:A:LYS:HG2	1:166:A:ARG:HD3	9	0.25
(1,1263)	1:163:A:LYS:HG3	1:166:A:ARG:HD2	9	0.25
(1,1263)	1:163:A:LYS:HG3	1:166:A:ARG:HD3	9	0.25
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	9	0.25
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	9	0.25
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	9	0.25
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	9	0.25
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	9	0.25
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	9	0.25
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	9	0.25
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	9	0.25
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	9	0.25
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	9	0.25
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	9	0.25
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	9	0.25
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	9	0.25
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	9	0.25
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	9	0.25
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	9	0.25
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	9	0.25
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	9	0.25
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	3	0.25
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	3	0.25
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	3	0.25
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	3	0.25
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	3	0.25
(1,844)	1:59:A:ASN:HB2	1:78:A:ILE:HD11	2	0.25
(1,844)	1:59:A:ASN:HB2	1:78:A:ILE:HD12	2	0.25
(1,844)	1:59:A:ASN:HB2	1:78:A:ILE:HD13	2	0.25
(1,769)	1:116:A:TYR:HD1	1:138:A:VAL:HG21	2	0.25
(1,769)	1:116:A:TYR:HD1	1:138:A:VAL:HG22	2	0.25
(1,769)	1:116:A:TYR:HD1	1:138:A:VAL:HG23	2	0.25
(1,769)	1:116:A:TYR:HD2	1:138:A:VAL:HG21	2	0.25
(1,769)	1:116:A:TYR:HD2	1:138:A:VAL:HG22	2	0.25
(1,769)	1:116:A:TYR:HD2	1:138:A:VAL:HG23	2	0.25
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB1	2	0.25
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB2	2	0.25
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB3	2	0.25
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB1	2	0.25
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB2	2	0.25
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB3	2	0.25
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB1	2	0.25
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB2	2	0.25
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB3	2	0.25
(1,614)	1:28:A:THR:HG21	1:32:A:LYS:HA	10	0.25
(1,614)	1:28:A:THR:HG22	1:32:A:LYS:HA	10	0.25
(1,614)	1:28:A:THR:HG23	1:32:A:LYS:HA	10	0.25
(1,457)	1:147:A:PRO:HG2	1:156:A:ILE:HA	7	0.25
(1,322)	1:96:A:ILE:HD11	1:115:A:MET:HA	5	0.25
(1,322)	1:96:A:ILE:HD12	1:115:A:MET:HA	5	0.25
(1,322)	1:96:A:ILE:HD13	1:115:A:MET:HA	5	0.25
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	2	0.25
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	2	0.25
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	2	0.25
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	8	0.25
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	8	0.25
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	8	0.25
(1,295)	1:137:A:THR:HG21	1:160:A:MET:HA	6	0.25
(1,295)	1:137:A:THR:HG22	1:160:A:MET:HA	6	0.25
(1,295)	1:137:A:THR:HG23	1:160:A:MET:HA	6	0.25
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE1	1	0.25
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE2	1	0.25
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE3	1	0.25
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG11	7	0.24
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG12	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG13	7	0.24
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG21	7	0.24
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG22	7	0.24
(1,1158)	1:112:A:PHE:HZ	1:153:A:VAL:HG23	7	0.24
(1,1141)	1:103:A:LEU:HD11	1:115:A:MET:HE1	6	0.24
(1,1141)	1:103:A:LEU:HD11	1:115:A:MET:HE2	6	0.24
(1,1141)	1:103:A:LEU:HD11	1:115:A:MET:HE3	6	0.24
(1,1141)	1:103:A:LEU:HD12	1:115:A:MET:HE1	6	0.24
(1,1141)	1:103:A:LEU:HD12	1:115:A:MET:HE2	6	0.24
(1,1141)	1:103:A:LEU:HD12	1:115:A:MET:HE3	6	0.24
(1,1141)	1:103:A:LEU:HD13	1:115:A:MET:HE1	6	0.24
(1,1141)	1:103:A:LEU:HD13	1:115:A:MET:HE2	6	0.24
(1,1141)	1:103:A:LEU:HD13	1:115:A:MET:HE3	6	0.24
(1,1141)	1:103:A:LEU:HD21	1:115:A:MET:HE1	6	0.24
(1,1141)	1:103:A:LEU:HD21	1:115:A:MET:HE2	6	0.24
(1,1141)	1:103:A:LEU:HD21	1:115:A:MET:HE3	6	0.24
(1,1141)	1:103:A:LEU:HD22	1:115:A:MET:HE1	6	0.24
(1,1141)	1:103:A:LEU:HD22	1:115:A:MET:HE2	6	0.24
(1,1141)	1:103:A:LEU:HD22	1:115:A:MET:HE3	6	0.24
(1,1141)	1:103:A:LEU:HD23	1:115:A:MET:HE1	6	0.24
(1,1141)	1:103:A:LEU:HD23	1:115:A:MET:HE2	6	0.24
(1,1141)	1:103:A:LEU:HD23	1:115:A:MET:HE3	6	0.24
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	9	0.24
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	9	0.24
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	9	0.24
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	9	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	8	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	8	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	8	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	8	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	8	0.24
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	8	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	8	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	8	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	8	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	8	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	8	0.24
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	8	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	8	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	8	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	8	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	8	0.24
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	8	0.24
(1,891)	1:28:A:THR:HG21	1:35:A:LEU:HD11	10	0.24
(1,891)	1:28:A:THR:HG21	1:35:A:LEU:HD12	10	0.24
(1,891)	1:28:A:THR:HG21	1:35:A:LEU:HD13	10	0.24
(1,891)	1:28:A:THR:HG21	1:35:A:LEU:HD21	10	0.24
(1,891)	1:28:A:THR:HG21	1:35:A:LEU:HD22	10	0.24
(1,891)	1:28:A:THR:HG21	1:35:A:LEU:HD23	10	0.24
(1,891)	1:28:A:THR:HG22	1:35:A:LEU:HD11	10	0.24
(1,891)	1:28:A:THR:HG22	1:35:A:LEU:HD12	10	0.24
(1,891)	1:28:A:THR:HG22	1:35:A:LEU:HD13	10	0.24
(1,891)	1:28:A:THR:HG22	1:35:A:LEU:HD21	10	0.24
(1,891)	1:28:A:THR:HG22	1:35:A:LEU:HD22	10	0.24
(1,891)	1:28:A:THR:HG22	1:35:A:LEU:HD23	10	0.24
(1,891)	1:28:A:THR:HG23	1:35:A:LEU:HD11	10	0.24
(1,891)	1:28:A:THR:HG23	1:35:A:LEU:HD12	10	0.24
(1,891)	1:28:A:THR:HG23	1:35:A:LEU:HD13	10	0.24
(1,891)	1:28:A:THR:HG23	1:35:A:LEU:HD21	10	0.24
(1,891)	1:28:A:THR:HG23	1:35:A:LEU:HD22	10	0.24
(1,891)	1:28:A:THR:HG23	1:35:A:LEU:HD23	10	0.24
(1,883)	1:26:A:GLY:HA2	1:32:A:LYS:HB2	5	0.24
(1,883)	1:26:A:GLY:HA2	1:32:A:LYS:HB3	5	0.24
(1,883)	1:26:A:GLY:HA3	1:32:A:LYS:HB2	5	0.24
(1,883)	1:26:A:GLY:HA3	1:32:A:LYS:HB3	5	0.24
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	2	0.24
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	2	0.24
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	2	0.24
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	2	0.24
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	2	0.24
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	2	0.24
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD11	3	0.24
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD12	3	0.24
(1,736)	1:74:A:GLU:HA	1:79:A:LEU:HD13	3	0.24
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	10	0.24
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	10	0.24
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	10	0.24
(1,501)	1:93:A:VAL:HB	1:157:A:ALA:HA	6	0.24
(1,475)	1:178:A:LYS:HB2	1:181:A:SER:HA	6	0.24
(1,475)	1:178:A:LYS:HB3	1:181:A:SER:HA	6	0.24
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG11	7	0.24
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG12	7	0.24
(1,382)	1:41:A:ASP:HB2	1:88:A:VAL:HG13	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	4	0.24
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	4	0.24
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	4	0.24
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	6	0.24
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	6	0.24
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	6	0.24
(1,270)	1:121:A:GLU:HA	1:124:A:LYS:HG2	9	0.24
(1,69)	1:57:A:GLY:H	1:58:A:VAL:H	1	0.24
(1,32)	1:104:A:LYS:H	1:107:A:GLY:H	5	0.24
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG2	2	0.23
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG3	2	0.23
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	7	0.23
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	7	0.23
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD2	2	0.23
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD3	2	0.23
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD2	2	0.23
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD3	2	0.23
(1,979)	1:53:A:ALA:HA	1:58:A:VAL:HG11	6	0.23
(1,979)	1:53:A:ALA:HA	1:58:A:VAL:HG12	6	0.23
(1,979)	1:53:A:ALA:HA	1:58:A:VAL:HG13	6	0.23
(1,979)	1:53:A:ALA:HA	1:58:A:VAL:HG21	6	0.23
(1,979)	1:53:A:ALA:HA	1:58:A:VAL:HG22	6	0.23
(1,979)	1:53:A:ALA:HA	1:58:A:VAL:HG23	6	0.23
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	6	0.23
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	6	0.23
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	6	0.23
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	6	0.23
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	6	0.23
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	6	0.23
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	6	0.23
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	6	0.23
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	6	0.23
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	6	0.23
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	6	0.23
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	6	0.23
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	6	0.23
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	6	0.23
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	6	0.23
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	6	0.23
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	6	0.23
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	6	0.23
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB1	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB2	3	0.23
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB3	3	0.23
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB1	3	0.23
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB2	3	0.23
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB3	3	0.23
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB1	3	0.23
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB2	3	0.23
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB3	3	0.23
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	5	0.23
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	5	0.23
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	5	0.23
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	5	0.23
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	5	0.23
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	5	0.23
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG21	9	0.23
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG22	9	0.23
(1,678)	1:30:A:ALA:HB1	1:33:A:ILE:HG23	9	0.23
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG21	9	0.23
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG22	9	0.23
(1,678)	1:30:A:ALA:HB2	1:33:A:ILE:HG23	9	0.23
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG21	9	0.23
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG22	9	0.23
(1,678)	1:30:A:ALA:HB3	1:33:A:ILE:HG23	9	0.23
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG21	4	0.23
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG22	4	0.23
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG23	4	0.23
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG21	4	0.23
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG22	4	0.23
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG23	4	0.23
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG21	4	0.23
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG22	4	0.23
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG23	4	0.23
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD11	1	0.23
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD12	1	0.23
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD13	1	0.23
(1,571)	1:52:A:ASP:HA	1:55:A:LEU:HB3	3	0.23
(1,550)	1:30:A:ALA:HB1	1:33:A:ILE:HB	1	0.23
(1,550)	1:30:A:ALA:HB2	1:33:A:ILE:HB	1	0.23
(1,550)	1:30:A:ALA:HB3	1:33:A:ILE:HB	1	0.23
(1,475)	1:178:A:LYS:HB2	1:181:A:SER:HA	5	0.23
(1,475)	1:178:A:LYS:HB3	1:181:A:SER:HA	5	0.23
(1,457)	1:147:A:PRO:HG2	1:156:A:ILE:HA	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:115:A:MET:HE1	1:118:A:LEU:HB2	6	0.23
(1,433)	1:115:A:MET:HE2	1:118:A:LEU:HB2	6	0.23
(1,433)	1:115:A:MET:HE3	1:118:A:LEU:HB2	6	0.23
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG21	2	0.23
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG22	2	0.23
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG23	2	0.23
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG21	2	0.23
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG22	2	0.23
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG23	2	0.23
(1,366)	1:142:A:ALA:HB1	1:146:A:PRO:HD2	8	0.23
(1,366)	1:142:A:ALA:HB2	1:146:A:PRO:HD2	8	0.23
(1,366)	1:142:A:ALA:HB3	1:146:A:PRO:HD2	8	0.23
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	7	0.23
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	7	0.23
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	7	0.23
(1,229)	1:174:A:THR:HB	1:175:A:LEU:HD21	4	0.23
(1,229)	1:174:A:THR:HB	1:175:A:LEU:HD22	4	0.23
(1,229)	1:174:A:THR:HB	1:175:A:LEU:HD23	4	0.23
(1,1290)	1:178:A:LYS:HB2	1:181:A:SER:HB2	10	0.22
(1,1290)	1:178:A:LYS:HB2	1:181:A:SER:HB3	10	0.22
(1,1290)	1:178:A:LYS:HB3	1:181:A:SER:HB2	10	0.22
(1,1290)	1:178:A:LYS:HB3	1:181:A:SER:HB3	10	0.22
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	1	0.22
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	1	0.22
(1,1085)	1:93:A:VAL:HB	1:164:A:LEU:HD11	9	0.22
(1,1085)	1:93:A:VAL:HB	1:164:A:LEU:HD12	9	0.22
(1,1085)	1:93:A:VAL:HB	1:164:A:LEU:HD13	9	0.22
(1,1085)	1:93:A:VAL:HB	1:164:A:LEU:HD21	9	0.22
(1,1085)	1:93:A:VAL:HB	1:164:A:LEU:HD22	9	0.22
(1,1085)	1:93:A:VAL:HB	1:164:A:LEU:HD23	9	0.22
(1,1051)	1:82:A:LYS:HA	1:167:A:VAL:HG11	5	0.22
(1,1051)	1:82:A:LYS:HA	1:167:A:VAL:HG12	5	0.22
(1,1051)	1:82:A:LYS:HA	1:167:A:VAL:HG13	5	0.22
(1,1051)	1:82:A:LYS:HA	1:167:A:VAL:HG21	5	0.22
(1,1051)	1:82:A:LYS:HA	1:167:A:VAL:HG22	5	0.22
(1,1051)	1:82:A:LYS:HA	1:167:A:VAL:HG23	5	0.22
(1,1048)	1:80:A:GLU:HB2	1:175:A:LEU:HD11	9	0.22
(1,1048)	1:80:A:GLU:HB2	1:175:A:LEU:HD12	9	0.22
(1,1048)	1:80:A:GLU:HB2	1:175:A:LEU:HD13	9	0.22
(1,1048)	1:80:A:GLU:HB2	1:175:A:LEU:HD21	9	0.22
(1,1048)	1:80:A:GLU:HB2	1:175:A:LEU:HD22	9	0.22
(1,1048)	1:80:A:GLU:HB2	1:175:A:LEU:HD23	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	1:80:A:GLU:HB3	1:175:A:LEU:HD11	9	0.22
(1,1048)	1:80:A:GLU:HB3	1:175:A:LEU:HD12	9	0.22
(1,1048)	1:80:A:GLU:HB3	1:175:A:LEU:HD13	9	0.22
(1,1048)	1:80:A:GLU:HB3	1:175:A:LEU:HD21	9	0.22
(1,1048)	1:80:A:GLU:HB3	1:175:A:LEU:HD22	9	0.22
(1,1048)	1:80:A:GLU:HB3	1:175:A:LEU:HD23	9	0.22
(1,1043)	1:79:A:LEU:HD11	1:82:A:LYS:HG2	5	0.22
(1,1043)	1:79:A:LEU:HD11	1:82:A:LYS:HG3	5	0.22
(1,1043)	1:79:A:LEU:HD12	1:82:A:LYS:HG2	5	0.22
(1,1043)	1:79:A:LEU:HD12	1:82:A:LYS:HG3	5	0.22
(1,1043)	1:79:A:LEU:HD13	1:82:A:LYS:HG2	5	0.22
(1,1043)	1:79:A:LEU:HD13	1:82:A:LYS:HG3	5	0.22
(1,1043)	1:79:A:LEU:HD21	1:82:A:LYS:HG2	5	0.22
(1,1043)	1:79:A:LEU:HD21	1:82:A:LYS:HG3	5	0.22
(1,1043)	1:79:A:LEU:HD22	1:82:A:LYS:HG2	5	0.22
(1,1043)	1:79:A:LEU:HD22	1:82:A:LYS:HG3	5	0.22
(1,1043)	1:79:A:LEU:HD23	1:82:A:LYS:HG2	5	0.22
(1,1043)	1:79:A:LEU:HD23	1:82:A:LYS:HG3	5	0.22
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	3	0.22
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	3	0.22
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	3	0.22
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	3	0.22
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	3	0.22
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	3	0.22
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	3	0.22
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	3	0.22
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	3	0.22
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	3	0.22
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	3	0.22
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	3	0.22
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	3	0.22
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	3	0.22
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	3	0.22
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	3	0.22
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	3	0.22
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	3	0.22
(1,907)	1:34:A:ARG:HA	1:37:A:ARG:HG2	2	0.22
(1,907)	1:34:A:ARG:HA	1:37:A:ARG:HG3	2	0.22
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD11	3	0.22
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD12	3	0.22
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD13	3	0.22
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD21	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD22	3	0.22
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD23	3	0.22
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	9	0.22
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	9	0.22
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	9	0.22
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	9	0.22
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	9	0.22
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	9	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB1	5	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB2	5	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB3	5	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB1	5	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB2	5	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB3	5	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB1	5	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB2	5	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB3	5	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB1	7	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB2	7	0.22
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB3	7	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB1	7	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB2	7	0.22
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB3	7	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB1	7	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB2	7	0.22
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB3	7	0.22
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	2	0.22
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	2	0.22
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	2	0.22
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	2	0.22
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	2	0.22
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	2	0.22
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	2	0.22
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	2	0.22
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	2	0.22
(1,540)	1:101:A:THR:HG21	1:154:A:LEU:HG	8	0.22
(1,540)	1:101:A:THR:HG22	1:154:A:LEU:HG	8	0.22
(1,540)	1:101:A:THR:HG23	1:154:A:LEU:HG	8	0.22
(1,540)	1:101:A:THR:HG21	1:154:A:LEU:HG	9	0.22
(1,540)	1:101:A:THR:HG22	1:154:A:LEU:HG	9	0.22
(1,540)	1:101:A:THR:HG23	1:154:A:LEU:HG	9	0.22
(1,510)	1:103:A:LEU:HB2	1:107:A:GLY:HA3	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:103:A:LEU:HB3	1:107:A:GLY:HA3	10	0.22
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG21	2	0.22
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG22	2	0.22
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG23	2	0.22
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG21	8	0.22
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG22	8	0.22
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG23	8	0.22
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE1	7	0.22
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE2	7	0.22
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE3	7	0.22
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE1	9	0.22
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE2	9	0.22
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE3	9	0.22
(1,194)	1:106:A:THR:H	1:107:A:GLY:H	5	0.22
(1,182)	1:105:A:GLU:H	1:106:A:THR:H	1	0.22
(1,1292)	1:183:A:PHE:HE1	1:185:A:ASP:HB2	2	0.21
(1,1292)	1:183:A:PHE:HE1	1:185:A:ASP:HB3	2	0.21
(1,1292)	1:183:A:PHE:HE2	1:185:A:ASP:HB2	2	0.21
(1,1292)	1:183:A:PHE:HE2	1:185:A:ASP:HB3	2	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	3	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	3	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	3	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	3	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	3	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	3	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	3	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	3	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	3	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	3	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	3	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	3	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	3	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	3	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	3	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	3	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	3	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	3	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	4	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	4	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	4	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	4	0.21
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	4	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	4	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	4	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	4	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	4	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	4	0.21
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	4	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	4	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	4	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	4	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	4	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	4	0.21
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	4	0.21
(1,1118)	1:96:A:ILE:HD11	1:153:A:VAL:HG11	5	0.21
(1,1118)	1:96:A:ILE:HD11	1:153:A:VAL:HG12	5	0.21
(1,1118)	1:96:A:ILE:HD11	1:153:A:VAL:HG13	5	0.21
(1,1118)	1:96:A:ILE:HD11	1:153:A:VAL:HG21	5	0.21
(1,1118)	1:96:A:ILE:HD11	1:153:A:VAL:HG22	5	0.21
(1,1118)	1:96:A:ILE:HD11	1:153:A:VAL:HG23	5	0.21
(1,1118)	1:96:A:ILE:HD12	1:153:A:VAL:HG11	5	0.21
(1,1118)	1:96:A:ILE:HD12	1:153:A:VAL:HG12	5	0.21
(1,1118)	1:96:A:ILE:HD12	1:153:A:VAL:HG13	5	0.21
(1,1118)	1:96:A:ILE:HD12	1:153:A:VAL:HG21	5	0.21
(1,1118)	1:96:A:ILE:HD12	1:153:A:VAL:HG22	5	0.21
(1,1118)	1:96:A:ILE:HD12	1:153:A:VAL:HG23	5	0.21
(1,1118)	1:96:A:ILE:HD13	1:153:A:VAL:HG11	5	0.21
(1,1118)	1:96:A:ILE:HD13	1:153:A:VAL:HG12	5	0.21
(1,1118)	1:96:A:ILE:HD13	1:153:A:VAL:HG13	5	0.21
(1,1118)	1:96:A:ILE:HD13	1:153:A:VAL:HG21	5	0.21
(1,1118)	1:96:A:ILE:HD13	1:153:A:VAL:HG22	5	0.21
(1,1118)	1:96:A:ILE:HD13	1:153:A:VAL:HG23	5	0.21
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG11	3	0.21
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG12	3	0.21
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG13	3	0.21
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG21	3	0.21
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG22	3	0.21
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG23	3	0.21
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG11	3	0.21
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG12	3	0.21
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG13	3	0.21
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG21	3	0.21
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG22	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG23	3	0.21
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG11	3	0.21
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG12	3	0.21
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG13	3	0.21
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG21	3	0.21
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG22	3	0.21
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG23	3	0.21
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	1	0.21
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	1	0.21
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	1	0.21
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	1	0.21
(1,888)	1:27:A:LEU:HD11	1:32:A:LYS:HA	7	0.21
(1,888)	1:27:A:LEU:HD12	1:32:A:LYS:HA	7	0.21
(1,888)	1:27:A:LEU:HD13	1:32:A:LYS:HA	7	0.21
(1,888)	1:27:A:LEU:HD21	1:32:A:LYS:HA	7	0.21
(1,888)	1:27:A:LEU:HD22	1:32:A:LYS:HA	7	0.21
(1,888)	1:27:A:LEU:HD23	1:32:A:LYS:HA	7	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD11	6	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD12	6	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD13	6	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD21	6	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD22	6	0.21
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD23	6	0.21
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	8	0.21
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	8	0.21
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	8	0.21
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	8	0.21
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	8	0.21
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	8	0.21
(1,649)	1:49:A:ILE:HG21	1:50:A:LYS:HG3	7	0.21
(1,649)	1:49:A:ILE:HG22	1:50:A:LYS:HG3	7	0.21
(1,649)	1:49:A:ILE:HG23	1:50:A:LYS:HG3	7	0.21
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	7	0.21
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	7	0.21
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	7	0.21
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	7	0.21
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	7	0.21
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	7	0.21
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	7	0.21
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	7	0.21
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	7	0.21
(1,538)	1:126:A:LEU:HD21	1:131:A:ILE:HB	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:126:A:LEU:HD22	1:131:A:ILE:HB	1	0.21
(1,538)	1:126:A:LEU:HD23	1:131:A:ILE:HB	1	0.21
(1,457)	1:147:A:PRO:HG2	1:156:A:ILE:HA	9	0.21
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	5	0.21
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	5	0.21
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	5	0.21
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE1	5	0.21
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE2	5	0.21
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE3	5	0.21
(1,182)	1:105:A:GLU:H	1:106:A:THR:H	6	0.21
(1,1276)	1:172:A:TYR:HB2	1:176:A:LYS:HG2	2	0.2
(1,1276)	1:172:A:TYR:HB2	1:176:A:LYS:HG3	2	0.2
(1,1276)	1:172:A:TYR:HB3	1:176:A:LYS:HG2	2	0.2
(1,1276)	1:172:A:TYR:HB3	1:176:A:LYS:HG3	2	0.2
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD11	7	0.2
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD12	7	0.2
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD13	7	0.2
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD21	7	0.2
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD22	7	0.2
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD23	7	0.2
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD11	7	0.2
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD12	7	0.2
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD13	7	0.2
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD21	7	0.2
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD22	7	0.2
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD23	7	0.2
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD11	7	0.2
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD12	7	0.2
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD13	7	0.2
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD21	7	0.2
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD22	7	0.2
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD23	7	0.2
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD11	7	0.2
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD12	7	0.2
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD13	7	0.2
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD21	7	0.2
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD22	7	0.2
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD23	7	0.2
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD11	7	0.2
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD12	7	0.2
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD13	7	0.2
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD21	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD22	7	0.2
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD23	7	0.2
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD11	7	0.2
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD12	7	0.2
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD13	7	0.2
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD21	7	0.2
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD22	7	0.2
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD23	7	0.2
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD11	4	0.2
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD12	4	0.2
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD13	4	0.2
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD21	4	0.2
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD22	4	0.2
(1,1021)	1:74:A:GLU:HA	1:79:A:LEU:HD23	4	0.2
(1,903)	1:32:A:LYS:HB2	1:35:A:LEU:HD11	5	0.2
(1,903)	1:32:A:LYS:HB2	1:35:A:LEU:HD12	5	0.2
(1,903)	1:32:A:LYS:HB2	1:35:A:LEU:HD13	5	0.2
(1,903)	1:32:A:LYS:HB2	1:35:A:LEU:HD21	5	0.2
(1,903)	1:32:A:LYS:HB2	1:35:A:LEU:HD22	5	0.2
(1,903)	1:32:A:LYS:HB2	1:35:A:LEU:HD23	5	0.2
(1,903)	1:32:A:LYS:HB3	1:35:A:LEU:HD11	5	0.2
(1,903)	1:32:A:LYS:HB3	1:35:A:LEU:HD12	5	0.2
(1,903)	1:32:A:LYS:HB3	1:35:A:LEU:HD13	5	0.2
(1,903)	1:32:A:LYS:HB3	1:35:A:LEU:HD21	5	0.2
(1,903)	1:32:A:LYS:HB3	1:35:A:LEU:HD22	5	0.2
(1,903)	1:32:A:LYS:HB3	1:35:A:LEU:HD23	5	0.2
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	3	0.2
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	3	0.2
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	3	0.2
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	3	0.2
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	3	0.2
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	3	0.2
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	4	0.2
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	4	0.2
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	4	0.2
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	4	0.2
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	4	0.2
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	4	0.2
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	4	0.2
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	4	0.2
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	4	0.2
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD11	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD12	4	0.2
(1,665)	1:115:A:MET:HA	1:118:A:LEU:HD13	4	0.2
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	5	0.2
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	5	0.2
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	5	0.2
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB2	7	0.2
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB3	7	0.2
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB2	7	0.2
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB3	7	0.2
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB2	7	0.2
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB3	7	0.2
(1,446)	1:131:A:ILE:HD11	1:167:A:VAL:HB	8	0.2
(1,446)	1:131:A:ILE:HD12	1:167:A:VAL:HB	8	0.2
(1,446)	1:131:A:ILE:HD13	1:167:A:VAL:HB	8	0.2
(1,393)	1:78:A:ILE:HG21	1:82:A:LYS:HE2	6	0.2
(1,393)	1:78:A:ILE:HG21	1:82:A:LYS:HE3	6	0.2
(1,393)	1:78:A:ILE:HG22	1:82:A:LYS:HE2	6	0.2
(1,393)	1:78:A:ILE:HG22	1:82:A:LYS:HE3	6	0.2
(1,393)	1:78:A:ILE:HG23	1:82:A:LYS:HE2	6	0.2
(1,393)	1:78:A:ILE:HG23	1:82:A:LYS:HE3	6	0.2
(1,390)	1:131:A:ILE:HG21	1:163:A:LYS:HE2	6	0.2
(1,390)	1:131:A:ILE:HG21	1:163:A:LYS:HE3	6	0.2
(1,390)	1:131:A:ILE:HG22	1:163:A:LYS:HE2	6	0.2
(1,390)	1:131:A:ILE:HG22	1:163:A:LYS:HE3	6	0.2
(1,390)	1:131:A:ILE:HG23	1:163:A:LYS:HE2	6	0.2
(1,390)	1:131:A:ILE:HG23	1:163:A:LYS:HE3	6	0.2
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	10	0.2
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	10	0.2
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	10	0.2
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	8	0.19
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	8	0.19
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	8	0.19
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	8	0.19
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	8	0.19
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	8	0.19
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	8	0.19
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	8	0.19
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	8	0.19
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	8	0.19
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	8	0.19
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	8	0.19
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	8	0.19
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	8	0.19
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	8	0.19
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	8	0.19
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	8	0.19
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	5	0.19
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	5	0.19
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	5	0.19
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	5	0.19
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	5	0.19
(1,966)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	5	0.19
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	5	0.19
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	5	0.19
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	5	0.19
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	5	0.19
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	5	0.19
(1,966)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	5	0.19
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	5	0.19
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	5	0.19
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	5	0.19
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	5	0.19
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	5	0.19
(1,966)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	5	0.19
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD11	5	0.19
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD12	5	0.19
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD13	5	0.19
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD21	5	0.19
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD22	5	0.19
(1,886)	1:27:A:LEU:HA	1:35:A:LEU:HD23	5	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE1	4	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE2	4	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE3	4	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE1	8	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE2	8	0.19
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE3	8	0.19
(1,833)	1:53:A:ALA:HB1	1:60:A:PHE:HZ	6	0.19
(1,833)	1:53:A:ALA:HB2	1:60:A:PHE:HZ	6	0.19
(1,833)	1:53:A:ALA:HB3	1:60:A:PHE:HZ	6	0.19
(1,811)	1:27:A:LEU:HB2	1:32:A:LYS:H	4	0.19
(1,811)	1:27:A:LEU:HB3	1:32:A:LYS:H	4	0.19
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	9	0.19
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	9	0.19
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	9	0.19
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	9	0.19
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	9	0.19
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	1	0.19
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	1	0.19
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	1	0.19
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	1	0.19
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	1	0.19
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	1	0.19
(1,757)	1:183:A:PHE:HE1	1:185:A:ASP:HB3	9	0.19
(1,757)	1:183:A:PHE:HE2	1:185:A:ASP:HB3	9	0.19
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD11	9	0.19
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD12	9	0.19
(1,705)	1:93:A:VAL:HG21	1:96:A:ILE:HD13	9	0.19
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD11	9	0.19
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD12	9	0.19
(1,705)	1:93:A:VAL:HG22	1:96:A:ILE:HD13	9	0.19
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD11	9	0.19
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD12	9	0.19
(1,705)	1:93:A:VAL:HG23	1:96:A:ILE:HD13	9	0.19
(1,649)	1:49:A:ILE:HG21	1:50:A:LYS:HG3	6	0.19
(1,649)	1:49:A:ILE:HG22	1:50:A:LYS:HG3	6	0.19
(1,649)	1:49:A:ILE:HG23	1:50:A:LYS:HG3	6	0.19
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD11	6	0.19
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD12	6	0.19
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD13	6	0.19
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD11	6	0.19
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD12	6	0.19
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD13	6	0.19
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD11	6	0.19
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD12	6	0.19
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD13	6	0.19
(1,614)	1:28:A:THR:HG21	1:32:A:LYS:HA	6	0.19
(1,614)	1:28:A:THR:HG22	1:32:A:LYS:HA	6	0.19
(1,614)	1:28:A:THR:HG23	1:32:A:LYS:HA	6	0.19
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	6	0.19
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	6	0.19
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	6	0.19
(1,588)	1:154:A:LEU:HG	1:157:A:ALA:HB1	3	0.19
(1,588)	1:154:A:LEU:HG	1:157:A:ALA:HB2	3	0.19
(1,588)	1:154:A:LEU:HG	1:157:A:ALA:HB3	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:30:A:ALA:HB1	1:33:A:ILE:HB	5	0.19
(1,550)	1:30:A:ALA:HB2	1:33:A:ILE:HB	5	0.19
(1,550)	1:30:A:ALA:HB3	1:33:A:ILE:HB	5	0.19
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	9	0.19
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	9	0.19
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	9	0.19
(1,518)	1:27:A:LEU:HG	1:32:A:LYS:HB2	10	0.19
(1,518)	1:27:A:LEU:HG	1:32:A:LYS:HB3	10	0.19
(1,423)	1:120:A:PHE:HB3	1:135:A:THR:HG21	1	0.19
(1,423)	1:120:A:PHE:HB3	1:135:A:THR:HG22	1	0.19
(1,423)	1:120:A:PHE:HB3	1:135:A:THR:HG23	1	0.19
(1,402)	1:59:A:ASN:HB2	1:62:A:ALA:HB1	2	0.19
(1,402)	1:59:A:ASN:HB2	1:62:A:ALA:HB2	2	0.19
(1,402)	1:59:A:ASN:HB2	1:62:A:ALA:HB3	2	0.19
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	5	0.19
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	5	0.19
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	5	0.19
(1,311)	1:94:A:ILE:HG21	1:95:A:ALA:HA	6	0.19
(1,311)	1:94:A:ILE:HG22	1:95:A:ALA:HA	6	0.19
(1,311)	1:94:A:ILE:HG23	1:95:A:ALA:HA	6	0.19
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	4	0.19
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	4	0.19
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	4	0.19
(1,295)	1:137:A:THR:HG21	1:160:A:MET:HA	1	0.19
(1,295)	1:137:A:THR:HG22	1:160:A:MET:HA	1	0.19
(1,295)	1:137:A:THR:HG23	1:160:A:MET:HA	1	0.19
(1,256)	1:147:A:PRO:HA	1:156:A:ILE:HD11	2	0.19
(1,256)	1:147:A:PRO:HA	1:156:A:ILE:HD12	2	0.19
(1,256)	1:147:A:PRO:HA	1:156:A:ILE:HD13	2	0.19
(1,47)	1:65:A:ASP:H	1:66:A:LYS:H	2	0.19
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG2	8	0.18
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG3	8	0.18
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG2	8	0.18
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG3	8	0.18
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG2	10	0.18
(1,1288)	1:177:A:LYS:HG2	1:178:A:LYS:HG3	10	0.18
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG2	10	0.18
(1,1288)	1:177:A:LYS:HG3	1:178:A:LYS:HG3	10	0.18
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE1	2	0.18
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE2	2	0.18
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE3	2	0.18
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE1	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE2	2	0.18
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE3	2	0.18
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE1	2	0.18
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE2	2	0.18
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE3	2	0.18
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE1	2	0.18
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE2	2	0.18
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE3	2	0.18
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE1	2	0.18
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE2	2	0.18
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE3	2	0.18
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE1	2	0.18
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE2	2	0.18
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE3	2	0.18
(1,1231)	1:140:A:ASP:HB2	1:143:A:GLU:HG2	7	0.18
(1,1231)	1:140:A:ASP:HB2	1:143:A:GLU:HG3	7	0.18
(1,1231)	1:140:A:ASP:HB3	1:143:A:GLU:HG2	7	0.18
(1,1231)	1:140:A:ASP:HB3	1:143:A:GLU:HG3	7	0.18
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB2	5	0.18
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB3	5	0.18
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB2	5	0.18
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB3	5	0.18
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB2	5	0.18
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB3	5	0.18
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	4	0.18
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	4	0.18
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	2	0.18
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	2	0.18
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	2	0.18
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	2	0.18
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	10	0.18
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	10	0.18
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	10	0.18
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	10	0.18
(1,595)	1:82:A:LYS:HG2	1:131:A:ILE:HA	5	0.18
(1,595)	1:82:A:LYS:HG3	1:131:A:ILE:HA	5	0.18
(1,558)	1:100:A:ALA:HB1	1:103:A:LEU:HG	10	0.18
(1,558)	1:100:A:ALA:HB2	1:103:A:LEU:HG	10	0.18
(1,558)	1:100:A:ALA:HB3	1:103:A:LEU:HG	10	0.18
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB1	10	0.18
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB2	10	0.18
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB1	10	0.18
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB2	10	0.18
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB3	10	0.18
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB1	10	0.18
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB2	10	0.18
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB3	10	0.18
(1,433)	1:115:A:MET:HE1	1:118:A:LEU:HB2	3	0.18
(1,433)	1:115:A:MET:HE2	1:118:A:LEU:HB2	3	0.18
(1,433)	1:115:A:MET:HE3	1:118:A:LEU:HB2	3	0.18
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	9	0.18
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	9	0.18
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	9	0.18
(1,329)	1:80:A:GLU:HA	1:175:A:LEU:HD11	4	0.18
(1,329)	1:80:A:GLU:HA	1:175:A:LEU:HD12	4	0.18
(1,329)	1:80:A:GLU:HA	1:175:A:LEU:HD13	4	0.18
(1,299)	1:141:A:ALA:HB1	1:155:A:GLU:HA	8	0.18
(1,299)	1:141:A:ALA:HB2	1:155:A:GLU:HA	8	0.18
(1,299)	1:141:A:ALA:HB3	1:155:A:GLU:HA	8	0.18
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE1	7	0.18
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE2	7	0.18
(1,244)	1:133:A:GLU:HA	1:134:A:MET:HE3	7	0.18
(1,206)	1:183:A:PHE:HA	1:186:A:GLU:HG3	1	0.18
(1,191)	1:28:A:THR:H	1:32:A:LYS:H	1	0.18
(1,56)	1:133:A:GLU:H	1:134:A:MET:H	4	0.18
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG2	9	0.17
(1,1280)	1:175:A:LEU:HA	1:177:A:LYS:HG3	9	0.17
(1,1262)	1:163:A:LYS:HG2	1:166:A:ARG:HB2	2	0.17
(1,1262)	1:163:A:LYS:HG2	1:166:A:ARG:HB3	2	0.17
(1,1262)	1:163:A:LYS:HG3	1:166:A:ARG:HB2	2	0.17
(1,1262)	1:163:A:LYS:HG3	1:166:A:ARG:HB3	2	0.17
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE1	9	0.17
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE2	9	0.17
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE3	9	0.17
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE1	9	0.17
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE2	9	0.17
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE3	9	0.17
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE1	9	0.17
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE2	9	0.17
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE3	9	0.17
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE1	9	0.17
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE2	9	0.17
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE3	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE1	9	0.17
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE2	9	0.17
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE3	9	0.17
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE1	9	0.17
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE2	9	0.17
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE3	9	0.17
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG11	2	0.17
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG12	2	0.17
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG13	2	0.17
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG21	2	0.17
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG22	2	0.17
(1,1233)	1:141:A:ALA:HB1	1:153:A:VAL:HG23	2	0.17
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG11	2	0.17
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG12	2	0.17
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG13	2	0.17
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG21	2	0.17
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG22	2	0.17
(1,1233)	1:141:A:ALA:HB2	1:153:A:VAL:HG23	2	0.17
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG11	2	0.17
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG12	2	0.17
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG13	2	0.17
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG21	2	0.17
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG22	2	0.17
(1,1233)	1:141:A:ALA:HB3	1:153:A:VAL:HG23	2	0.17
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD11	8	0.17
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD12	8	0.17
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD13	8	0.17
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD21	8	0.17
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD22	8	0.17
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD23	8	0.17
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD11	1	0.17
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD12	1	0.17
(1,847)	1:63:A:PHE:HA	1:78:A:ILE:HD13	1	0.17
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	5	0.17
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	5	0.17
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	5	0.17
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	5	0.17
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	5	0.17
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	5	0.17
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD11	3	0.17
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD12	3	0.17
(1,648)	1:46:A:ILE:HG21	1:126:A:LEU:HD13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD11	3	0.17
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD12	3	0.17
(1,648)	1:46:A:ILE:HG22	1:126:A:LEU:HD13	3	0.17
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD11	3	0.17
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD12	3	0.17
(1,648)	1:46:A:ILE:HG23	1:126:A:LEU:HD13	3	0.17
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD11	6	0.17
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD12	6	0.17
(1,574)	1:91:A:LYS:HG3	1:94:A:ILE:HD13	6	0.17
(1,558)	1:100:A:ALA:HB1	1:103:A:LEU:HG	4	0.17
(1,558)	1:100:A:ALA:HB2	1:103:A:LEU:HG	4	0.17
(1,558)	1:100:A:ALA:HB3	1:103:A:LEU:HG	4	0.17
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB1	6	0.17
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB2	6	0.17
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB3	6	0.17
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB1	6	0.17
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB2	6	0.17
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB3	6	0.17
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB1	6	0.17
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB2	6	0.17
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB3	6	0.17
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB2	5	0.17
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB3	5	0.17
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB2	5	0.17
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB3	5	0.17
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB2	5	0.17
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB3	5	0.17
(1,461)	1:31:A:THR:HG21	1:99:A:GLU:HB2	3	0.17
(1,461)	1:31:A:THR:HG21	1:99:A:GLU:HB3	3	0.17
(1,461)	1:31:A:THR:HG22	1:99:A:GLU:HB2	3	0.17
(1,461)	1:31:A:THR:HG22	1:99:A:GLU:HB3	3	0.17
(1,461)	1:31:A:THR:HG23	1:99:A:GLU:HB2	3	0.17
(1,461)	1:31:A:THR:HG23	1:99:A:GLU:HB3	3	0.17
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD11	10	0.17
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD12	10	0.17
(1,413)	1:76:A:PRO:HB2	1:175:A:LEU:HD13	10	0.17
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD11	10	0.17
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD12	10	0.17
(1,413)	1:76:A:PRO:HB3	1:175:A:LEU:HD13	10	0.17
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG21	4	0.17
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG22	4	0.17
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG23	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:33:A:ILE:HG21	1:34:A:ARG:HA	1	0.17
(1,315)	1:33:A:ILE:HG22	1:34:A:ARG:HA	1	0.17
(1,315)	1:33:A:ILE:HG23	1:34:A:ARG:HA	1	0.17
(1,313)	1:42:A:ILE:HG21	1:126:A:LEU:HA	8	0.17
(1,313)	1:42:A:ILE:HG22	1:126:A:LEU:HA	8	0.17
(1,313)	1:42:A:ILE:HG23	1:126:A:LEU:HA	8	0.17
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE1	7	0.16
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE2	7	0.16
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE3	7	0.16
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE1	7	0.16
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE2	7	0.16
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE3	7	0.16
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE1	7	0.16
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE2	7	0.16
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE3	7	0.16
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE1	7	0.16
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE2	7	0.16
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE3	7	0.16
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE1	7	0.16
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE2	7	0.16
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE3	7	0.16
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE1	7	0.16
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE2	7	0.16
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE3	7	0.16
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB2	4	0.16
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB3	4	0.16
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB2	4	0.16
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB3	4	0.16
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB2	4	0.16
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB3	4	0.16
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG21	4	0.16
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG22	4	0.16
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG23	4	0.16
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG21	4	0.16
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG22	4	0.16
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG23	4	0.16
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD11	4	0.16
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD12	4	0.16
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD13	4	0.16
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD21	4	0.16
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD22	4	0.16
(1,1144)	1:103:A:LEU:HD11	1:154:A:LEU:HD23	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD11	4	0.16
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD12	4	0.16
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD13	4	0.16
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD21	4	0.16
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD22	4	0.16
(1,1144)	1:103:A:LEU:HD12	1:154:A:LEU:HD23	4	0.16
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD11	4	0.16
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD12	4	0.16
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD13	4	0.16
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD21	4	0.16
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD22	4	0.16
(1,1144)	1:103:A:LEU:HD13	1:154:A:LEU:HD23	4	0.16
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD11	4	0.16
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD12	4	0.16
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD13	4	0.16
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD21	4	0.16
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD22	4	0.16
(1,1144)	1:103:A:LEU:HD21	1:154:A:LEU:HD23	4	0.16
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD11	4	0.16
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD12	4	0.16
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD13	4	0.16
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD21	4	0.16
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD22	4	0.16
(1,1144)	1:103:A:LEU:HD22	1:154:A:LEU:HD23	4	0.16
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD11	4	0.16
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD12	4	0.16
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD13	4	0.16
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD21	4	0.16
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD22	4	0.16
(1,1144)	1:103:A:LEU:HD23	1:154:A:LEU:HD23	4	0.16
(1,1059)	1:83:A:VAL:HG11	1:169:A:THR:HA	4	0.16
(1,1059)	1:83:A:VAL:HG12	1:169:A:THR:HA	4	0.16
(1,1059)	1:83:A:VAL:HG13	1:169:A:THR:HA	4	0.16
(1,1059)	1:83:A:VAL:HG21	1:169:A:THR:HA	4	0.16
(1,1059)	1:83:A:VAL:HG22	1:169:A:THR:HA	4	0.16
(1,1059)	1:83:A:VAL:HG23	1:169:A:THR:HA	4	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD11	1	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD12	1	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD13	1	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD21	1	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD22	1	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD23	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD11	1	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD12	1	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD13	1	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD21	1	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD22	1	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD23	1	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD11	8	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD12	8	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD13	8	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD21	8	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD22	8	0.16
(1,1020)	1:73:A:SER:HB2	1:79:A:LEU:HD23	8	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD11	8	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD12	8	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD13	8	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD21	8	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD22	8	0.16
(1,1020)	1:73:A:SER:HB3	1:79:A:LEU:HD23	8	0.16
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	3	0.16
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	3	0.16
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	3	0.16
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	3	0.16
(1,914)	1:35:A:LEU:HB2	1:95:A:ALA:HB1	2	0.16
(1,914)	1:35:A:LEU:HB2	1:95:A:ALA:HB2	2	0.16
(1,914)	1:35:A:LEU:HB2	1:95:A:ALA:HB3	2	0.16
(1,914)	1:35:A:LEU:HB3	1:95:A:ALA:HB1	2	0.16
(1,914)	1:35:A:LEU:HB3	1:95:A:ALA:HB2	2	0.16
(1,914)	1:35:A:LEU:HB3	1:95:A:ALA:HB3	2	0.16
(1,756)	1:183:A:PHE:HE1	1:185:A:ASP:HB2	1	0.16
(1,756)	1:183:A:PHE:HE2	1:185:A:ASP:HB2	1	0.16
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD11	5	0.16
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD12	5	0.16
(1,726)	1:62:A:ALA:HB1	1:78:A:ILE:HD13	5	0.16
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD11	5	0.16
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD12	5	0.16
(1,726)	1:62:A:ALA:HB2	1:78:A:ILE:HD13	5	0.16
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD11	5	0.16
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD12	5	0.16
(1,726)	1:62:A:ALA:HB3	1:78:A:ILE:HD13	5	0.16
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB1	8	0.16
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB2	8	0.16
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB3	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB1	8	0.16
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB2	8	0.16
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB3	8	0.16
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB1	8	0.16
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB2	8	0.16
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB3	8	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB1	4	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB2	4	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB3	4	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB1	4	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB2	4	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB3	4	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB1	4	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB2	4	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB3	4	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB1	7	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB2	7	0.16
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB3	7	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB1	7	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB2	7	0.16
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB3	7	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB1	7	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB2	7	0.16
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB3	7	0.16
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE1	8	0.16
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE2	8	0.16
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE3	8	0.16
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE1	8	0.16
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE2	8	0.16
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE3	8	0.16
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE1	8	0.16
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE2	8	0.16
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE3	8	0.16
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	8	0.16
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	8	0.16
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	8	0.16
(1,526)	1:126:A:LEU:HD11	1:131:A:ILE:HB	4	0.16
(1,526)	1:126:A:LEU:HD12	1:131:A:ILE:HB	4	0.16
(1,526)	1:126:A:LEU:HD13	1:131:A:ILE:HB	4	0.16
(1,510)	1:103:A:LEU:HB2	1:107:A:GLY:HA3	4	0.16
(1,510)	1:103:A:LEU:HB3	1:107:A:GLY:HA3	4	0.16
(1,433)	1:115:A:MET:HE1	1:118:A:LEU:HB2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:115:A:MET:HE2	1:118:A:LEU:HB2	5	0.16
(1,433)	1:115:A:MET:HE3	1:118:A:LEU:HB2	5	0.16
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE1	10	0.16
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE2	10	0.16
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE3	10	0.16
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG21	10	0.16
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG22	10	0.16
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG23	10	0.16
(1,313)	1:42:A:ILE:HG21	1:126:A:LEU:HA	1	0.16
(1,313)	1:42:A:ILE:HG22	1:126:A:LEU:HA	1	0.16
(1,313)	1:42:A:ILE:HG23	1:126:A:LEU:HA	1	0.16
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	10	0.16
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	10	0.16
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	10	0.16
(1,299)	1:141:A:ALA:HB1	1:155:A:GLU:HA	2	0.16
(1,299)	1:141:A:ALA:HB2	1:155:A:GLU:HA	2	0.16
(1,299)	1:141:A:ALA:HB3	1:155:A:GLU:HA	2	0.16
(1,295)	1:137:A:THR:HG21	1:160:A:MET:HA	9	0.16
(1,295)	1:137:A:THR:HG22	1:160:A:MET:HA	9	0.16
(1,295)	1:137:A:THR:HG23	1:160:A:MET:HA	9	0.16
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG21	6	0.16
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG22	6	0.16
(1,289)	1:104:A:LYS:HA	1:106:A:THR:HG23	6	0.16
(1,205)	1:183:A:PHE:HA	1:186:A:GLU:HG2	9	0.16
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG11	9	0.15
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG12	9	0.15
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG13	9	0.15
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG21	9	0.15
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG22	9	0.15
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG23	9	0.15
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB2	3	0.15
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB3	3	0.15
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB2	3	0.15
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB3	3	0.15
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB2	3	0.15
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB3	3	0.15
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG21	2	0.15
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG22	2	0.15
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG23	2	0.15
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG21	2	0.15
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG22	2	0.15
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG23	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	9	0.15
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	9	0.15
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	9	0.15
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	9	0.15
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	9	0.15
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	9	0.15
(1,907)	1:34:A:ARG:HA	1:37:A:ARG:HG2	7	0.15
(1,907)	1:34:A:ARG:HA	1:37:A:ARG:HG3	7	0.15
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB1	5	0.15
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB2	5	0.15
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB3	5	0.15
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB1	5	0.15
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB2	5	0.15
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB3	5	0.15
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB1	5	0.15
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB2	5	0.15
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB3	5	0.15
(1,840)	1:63:A:PHE:HD1	1:67:A:LYS:HA	7	0.15
(1,840)	1:63:A:PHE:HD2	1:67:A:LYS:HA	7	0.15
(1,833)	1:53:A:ALA:HB1	1:60:A:PHE:HZ	4	0.15
(1,833)	1:53:A:ALA:HB2	1:60:A:PHE:HZ	4	0.15
(1,833)	1:53:A:ALA:HB3	1:60:A:PHE:HZ	4	0.15
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD11	6	0.15
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD12	6	0.15
(1,804)	1:116:A:TYR:HD1	1:156:A:ILE:HD13	6	0.15
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD11	6	0.15
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD12	6	0.15
(1,804)	1:116:A:TYR:HD2	1:156:A:ILE:HD13	6	0.15
(1,757)	1:183:A:PHE:HE1	1:185:A:ASP:HB3	7	0.15
(1,757)	1:183:A:PHE:HE2	1:185:A:ASP:HB3	7	0.15
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG21	1	0.15
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG22	1	0.15
(1,715)	1:46:A:ILE:HD11	1:88:A:VAL:HG23	1	0.15
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG21	1	0.15
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG22	1	0.15
(1,715)	1:46:A:ILE:HD12	1:88:A:VAL:HG23	1	0.15
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG21	1	0.15
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG22	1	0.15
(1,715)	1:46:A:ILE:HD13	1:88:A:VAL:HG23	1	0.15
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG21	9	0.15
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG22	9	0.15
(1,608)	1:85:A:ALA:HB1	1:131:A:ILE:HG23	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG21	9	0.15
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG22	9	0.15
(1,608)	1:85:A:ALA:HB2	1:131:A:ILE:HG23	9	0.15
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG21	9	0.15
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG22	9	0.15
(1,608)	1:85:A:ALA:HB3	1:131:A:ILE:HG23	9	0.15
(1,508)	1:96:A:ILE:HD11	1:118:A:LEU:HG	6	0.15
(1,508)	1:96:A:ILE:HD12	1:118:A:LEU:HG	6	0.15
(1,508)	1:96:A:ILE:HD13	1:118:A:LEU:HG	6	0.15
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB1	8	0.15
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB2	8	0.15
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB3	8	0.15
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB1	8	0.15
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB2	8	0.15
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB3	8	0.15
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB1	8	0.15
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB2	8	0.15
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB3	8	0.15
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	9	0.15
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	9	0.15
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	9	0.15
(1,318)	1:126:A:LEU:HA	1:131:A:ILE:HD11	3	0.15
(1,318)	1:126:A:LEU:HA	1:131:A:ILE:HD12	3	0.15
(1,318)	1:126:A:LEU:HA	1:131:A:ILE:HD13	3	0.15
(1,313)	1:42:A:ILE:HG21	1:126:A:LEU:HA	4	0.15
(1,313)	1:42:A:ILE:HG22	1:126:A:LEU:HA	4	0.15
(1,313)	1:42:A:ILE:HG23	1:126:A:LEU:HA	4	0.15
(1,270)	1:121:A:GLU:HA	1:124:A:LYS:HG2	1	0.15
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE1	6	0.15
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE2	6	0.15
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE3	6	0.15
(1,159)	1:144:A:GLU:H	1:145:A:ASN:H	3	0.15
(1,24)	1:150:A:ALA:H	1:153:A:VAL:H	1	0.15
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG11	7	0.14
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG12	7	0.14
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG13	7	0.14
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG21	7	0.14
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG22	7	0.14
(1,1225)	1:138:A:VAL:HG11	1:153:A:VAL:HG23	7	0.14
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG11	7	0.14
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG12	7	0.14
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG13	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG21	7	0.14
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG22	7	0.14
(1,1225)	1:138:A:VAL:HG12	1:153:A:VAL:HG23	7	0.14
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG11	7	0.14
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG12	7	0.14
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG13	7	0.14
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG21	7	0.14
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG22	7	0.14
(1,1225)	1:138:A:VAL:HG13	1:153:A:VAL:HG23	7	0.14
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG11	7	0.14
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG12	7	0.14
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG13	7	0.14
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG21	7	0.14
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG22	7	0.14
(1,1225)	1:138:A:VAL:HG21	1:153:A:VAL:HG23	7	0.14
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG11	7	0.14
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG12	7	0.14
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG13	7	0.14
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG21	7	0.14
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG22	7	0.14
(1,1225)	1:138:A:VAL:HG22	1:153:A:VAL:HG23	7	0.14
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG11	7	0.14
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG12	7	0.14
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG13	7	0.14
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG21	7	0.14
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG22	7	0.14
(1,1225)	1:138:A:VAL:HG23	1:153:A:VAL:HG23	7	0.14
(1,1216)	1:133:A:GLU:HG2	1:137:A:THR:HG21	6	0.14
(1,1216)	1:133:A:GLU:HG2	1:137:A:THR:HG22	6	0.14
(1,1216)	1:133:A:GLU:HG2	1:137:A:THR:HG23	6	0.14
(1,1216)	1:133:A:GLU:HG3	1:137:A:THR:HG21	6	0.14
(1,1216)	1:133:A:GLU:HG3	1:137:A:THR:HG22	6	0.14
(1,1216)	1:133:A:GLU:HG3	1:137:A:THR:HG23	6	0.14
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB2	8	0.14
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB3	8	0.14
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB2	8	0.14
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB3	8	0.14
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB2	8	0.14
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB3	8	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD11	8	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD12	8	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD13	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD21	8	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD22	8	0.14
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD23	8	0.14
(1,999)	1:59:A:ASN:HB2	1:62:A:ALA:HB1	2	0.14
(1,999)	1:59:A:ASN:HB2	1:62:A:ALA:HB2	2	0.14
(1,999)	1:59:A:ASN:HB2	1:62:A:ALA:HB3	2	0.14
(1,999)	1:59:A:ASN:HB3	1:62:A:ALA:HB1	2	0.14
(1,999)	1:59:A:ASN:HB3	1:62:A:ALA:HB2	2	0.14
(1,999)	1:59:A:ASN:HB3	1:62:A:ALA:HB3	2	0.14
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD2	9	0.14
(1,986)	1:55:A:LEU:HB2	1:56:A:LYS:HD3	9	0.14
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD2	9	0.14
(1,986)	1:55:A:LEU:HB3	1:56:A:LYS:HD3	9	0.14
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB1	10	0.14
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB2	10	0.14
(1,843)	1:78:A:ILE:HD11	1:81:A:ALA:HB3	10	0.14
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB1	10	0.14
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB2	10	0.14
(1,843)	1:78:A:ILE:HD12	1:81:A:ALA:HB3	10	0.14
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB1	10	0.14
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB2	10	0.14
(1,843)	1:78:A:ILE:HD13	1:81:A:ALA:HB3	10	0.14
(1,810)	1:63:A:PHE:HE1	1:78:A:ILE:HD11	5	0.14
(1,810)	1:63:A:PHE:HE1	1:78:A:ILE:HD12	5	0.14
(1,810)	1:63:A:PHE:HE1	1:78:A:ILE:HD13	5	0.14
(1,810)	1:63:A:PHE:HE2	1:78:A:ILE:HD11	5	0.14
(1,810)	1:63:A:PHE:HE2	1:78:A:ILE:HD12	5	0.14
(1,810)	1:63:A:PHE:HE2	1:78:A:ILE:HD13	5	0.14
(1,783)	1:112:A:PHE:HZ	1:115:A:MET:HE1	1	0.14
(1,783)	1:112:A:PHE:HZ	1:115:A:MET:HE2	1	0.14
(1,783)	1:112:A:PHE:HZ	1:115:A:MET:HE3	1	0.14
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	2	0.14
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	2	0.14
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	2	0.14
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	2	0.14
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	2	0.14
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	2	0.14
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE1	10	0.14
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE2	10	0.14
(1,782)	1:92:A:PHE:HD1	1:160:A:MET:HE3	10	0.14
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE1	10	0.14
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:92:A:PHE:HD2	1:160:A:MET:HE3	10	0.14
(1,770)	1:116:A:TYR:HD1	1:138:A:VAL:HG11	7	0.14
(1,770)	1:116:A:TYR:HD1	1:138:A:VAL:HG12	7	0.14
(1,770)	1:116:A:TYR:HD1	1:138:A:VAL:HG13	7	0.14
(1,770)	1:116:A:TYR:HD2	1:138:A:VAL:HG11	7	0.14
(1,770)	1:116:A:TYR:HD2	1:138:A:VAL:HG12	7	0.14
(1,770)	1:116:A:TYR:HD2	1:138:A:VAL:HG13	7	0.14
(1,758)	1:82:A:LYS:HE2	1:131:A:ILE:H	6	0.14
(1,758)	1:82:A:LYS:HE3	1:131:A:ILE:H	6	0.14
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG21	8	0.14
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG22	8	0.14
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG23	8	0.14
(1,653)	1:86:A:THR:HG21	1:131:A:ILE:HG12	3	0.14
(1,653)	1:86:A:THR:HG21	1:131:A:ILE:HG13	3	0.14
(1,653)	1:86:A:THR:HG22	1:131:A:ILE:HG12	3	0.14
(1,653)	1:86:A:THR:HG22	1:131:A:ILE:HG13	3	0.14
(1,653)	1:86:A:THR:HG23	1:131:A:ILE:HG12	3	0.14
(1,653)	1:86:A:THR:HG23	1:131:A:ILE:HG13	3	0.14
(1,631)	1:46:A:ILE:HD11	1:86:A:THR:HG21	8	0.14
(1,631)	1:46:A:ILE:HD11	1:86:A:THR:HG22	8	0.14
(1,631)	1:46:A:ILE:HD11	1:86:A:THR:HG23	8	0.14
(1,631)	1:46:A:ILE:HD12	1:86:A:THR:HG21	8	0.14
(1,631)	1:46:A:ILE:HD12	1:86:A:THR:HG22	8	0.14
(1,631)	1:46:A:ILE:HD12	1:86:A:THR:HG23	8	0.14
(1,631)	1:46:A:ILE:HD13	1:86:A:THR:HG21	8	0.14
(1,631)	1:46:A:ILE:HD13	1:86:A:THR:HG22	8	0.14
(1,631)	1:46:A:ILE:HD13	1:86:A:THR:HG23	8	0.14
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB1	3	0.14
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB2	3	0.14
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB3	3	0.14
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB1	3	0.14
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB2	3	0.14
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB3	3	0.14
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB1	3	0.14
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB2	3	0.14
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB3	3	0.14
(1,584)	1:101:A:THR:HG21	1:104:A:LYS:HB3	6	0.14
(1,584)	1:101:A:THR:HG22	1:104:A:LYS:HB3	6	0.14
(1,584)	1:101:A:THR:HG23	1:104:A:LYS:HB3	6	0.14
(1,540)	1:101:A:THR:HG21	1:154:A:LEU:HG	5	0.14
(1,540)	1:101:A:THR:HG22	1:154:A:LEU:HG	5	0.14
(1,540)	1:101:A:THR:HG23	1:154:A:LEU:HG	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:175:A:LEU:HB2	1:176:A:LYS:HE2	10	0.14
(1,512)	1:175:A:LEU:HB3	1:176:A:LYS:HE2	10	0.14
(1,457)	1:147:A:PRO:HG2	1:156:A:ILE:HA	2	0.14
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG21	5	0.14
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG22	5	0.14
(1,406)	1:67:A:LYS:HE2	1:78:A:ILE:HG23	5	0.14
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG21	5	0.14
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG22	5	0.14
(1,406)	1:67:A:LYS:HE3	1:78:A:ILE:HG23	5	0.14
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE1	2	0.14
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE2	2	0.14
(1,364)	1:116:A:TYR:HB2	1:160:A:MET:HE3	2	0.14
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	3	0.14
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	3	0.14
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	3	0.14
(1,299)	1:141:A:ALA:HB1	1:155:A:GLU:HA	4	0.14
(1,299)	1:141:A:ALA:HB2	1:155:A:GLU:HA	4	0.14
(1,299)	1:141:A:ALA:HB3	1:155:A:GLU:HA	4	0.14
(1,299)	1:141:A:ALA:HB1	1:155:A:GLU:HA	10	0.14
(1,299)	1:141:A:ALA:HB2	1:155:A:GLU:HA	10	0.14
(1,299)	1:141:A:ALA:HB3	1:155:A:GLU:HA	10	0.14
(1,247)	1:112:A:PHE:HA	1:115:A:MET:HE1	5	0.14
(1,247)	1:112:A:PHE:HA	1:115:A:MET:HE2	5	0.14
(1,247)	1:112:A:PHE:HA	1:115:A:MET:HE3	5	0.14
(1,226)	1:86:A:THR:HG21	1:165:A:GLN:HA	6	0.14
(1,226)	1:86:A:THR:HG22	1:165:A:GLN:HA	6	0.14
(1,226)	1:86:A:THR:HG23	1:165:A:GLN:HA	6	0.14
(1,69)	1:57:A:GLY:H	1:58:A:VAL:H	9	0.14
(1,1263)	1:163:A:LYS:HG2	1:166:A:ARG:HD2	10	0.13
(1,1263)	1:163:A:LYS:HG2	1:166:A:ARG:HD3	10	0.13
(1,1263)	1:163:A:LYS:HG3	1:166:A:ARG:HD2	10	0.13
(1,1263)	1:163:A:LYS:HG3	1:166:A:ARG:HD3	10	0.13
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE1	8	0.13
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE2	8	0.13
(1,1251)	1:153:A:VAL:HG11	1:160:A:MET:HE3	8	0.13
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE1	8	0.13
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE2	8	0.13
(1,1251)	1:153:A:VAL:HG12	1:160:A:MET:HE3	8	0.13
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE1	8	0.13
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE2	8	0.13
(1,1251)	1:153:A:VAL:HG13	1:160:A:MET:HE3	8	0.13
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE1	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE2	8	0.13
(1,1251)	1:153:A:VAL:HG21	1:160:A:MET:HE3	8	0.13
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE1	8	0.13
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE2	8	0.13
(1,1251)	1:153:A:VAL:HG22	1:160:A:MET:HE3	8	0.13
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE1	8	0.13
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE2	8	0.13
(1,1251)	1:153:A:VAL:HG23	1:160:A:MET:HE3	8	0.13
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG11	8	0.13
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG12	8	0.13
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG13	8	0.13
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG21	8	0.13
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG22	8	0.13
(1,1236)	1:147:A:PRO:HA	1:153:A:VAL:HG23	8	0.13
(1,1205)	1:131:A:ILE:HG21	1:163:A:LYS:HG2	10	0.13
(1,1205)	1:131:A:ILE:HG21	1:163:A:LYS:HG3	10	0.13
(1,1205)	1:131:A:ILE:HG22	1:163:A:LYS:HG2	10	0.13
(1,1205)	1:131:A:ILE:HG22	1:163:A:LYS:HG3	10	0.13
(1,1205)	1:131:A:ILE:HG23	1:163:A:LYS:HG2	10	0.13
(1,1205)	1:131:A:ILE:HG23	1:163:A:LYS:HG3	10	0.13
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB2	9	0.13
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB3	9	0.13
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB2	9	0.13
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB3	9	0.13
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB2	9	0.13
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB3	9	0.13
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB2	10	0.13
(1,1183)	1:119:A:MET:HE1	1:120:A:PHE:HB3	10	0.13
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB2	10	0.13
(1,1183)	1:119:A:MET:HE2	1:120:A:PHE:HB3	10	0.13
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB2	10	0.13
(1,1183)	1:119:A:MET:HE3	1:120:A:PHE:HB3	10	0.13
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD11	9	0.13
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD12	9	0.13
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD13	9	0.13
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD21	9	0.13
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD22	9	0.13
(1,1162)	1:115:A:MET:HA	1:118:A:LEU:HD23	9	0.13
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB2	3	0.13
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB3	3	0.13
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB2	3	0.13
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB2	3	0.13
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB3	3	0.13
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB2	9	0.13
(1,1129)	1:100:A:ALA:HB1	1:104:A:LYS:HB3	9	0.13
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB2	9	0.13
(1,1129)	1:100:A:ALA:HB2	1:104:A:LYS:HB3	9	0.13
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB2	9	0.13
(1,1129)	1:100:A:ALA:HB3	1:104:A:LYS:HB3	9	0.13
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD11	2	0.13
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD12	2	0.13
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD13	2	0.13
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD21	2	0.13
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD22	2	0.13
(1,1113)	1:96:A:ILE:HB	1:118:A:LEU:HD23	2	0.13
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG2	8	0.13
(1,1017)	1:71:A:GLY:HA2	1:80:A:GLU:HG3	8	0.13
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG2	8	0.13
(1,1017)	1:71:A:GLY:HA3	1:80:A:GLU:HG3	8	0.13
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD11	3	0.13
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD12	3	0.13
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD13	3	0.13
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD21	3	0.13
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD22	3	0.13
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD23	3	0.13
(1,934)	1:41:A:ASP:HA	1:88:A:VAL:HG11	8	0.13
(1,934)	1:41:A:ASP:HA	1:88:A:VAL:HG12	8	0.13
(1,934)	1:41:A:ASP:HA	1:88:A:VAL:HG13	8	0.13
(1,934)	1:41:A:ASP:HA	1:88:A:VAL:HG21	8	0.13
(1,934)	1:41:A:ASP:HA	1:88:A:VAL:HG22	8	0.13
(1,934)	1:41:A:ASP:HA	1:88:A:VAL:HG23	8	0.13
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB1	2	0.13
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB2	2	0.13
(1,884)	1:26:A:GLY:HA2	1:114:A:ALA:HB3	2	0.13
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB1	2	0.13
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB2	2	0.13
(1,884)	1:26:A:GLY:HA3	1:114:A:ALA:HB3	2	0.13
(1,833)	1:53:A:ALA:HB1	1:60:A:PHE:HZ	2	0.13
(1,833)	1:53:A:ALA:HB2	1:60:A:PHE:HZ	2	0.13
(1,833)	1:53:A:ALA:HB3	1:60:A:PHE:HZ	2	0.13
(1,833)	1:53:A:ALA:HB1	1:60:A:PHE:HZ	5	0.13
(1,833)	1:53:A:ALA:HB2	1:60:A:PHE:HZ	5	0.13
(1,833)	1:53:A:ALA:HB3	1:60:A:PHE:HZ	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	8	0.13
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	8	0.13
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	8	0.13
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	8	0.13
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	8	0.13
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	8	0.13
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	8	0.13
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	8	0.13
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	8	0.13
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE1	4	0.13
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE2	4	0.13
(1,600)	1:157:A:ALA:HB1	1:160:A:MET:HE3	4	0.13
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE1	4	0.13
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE2	4	0.13
(1,600)	1:157:A:ALA:HB2	1:160:A:MET:HE3	4	0.13
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE1	4	0.13
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE2	4	0.13
(1,600)	1:157:A:ALA:HB3	1:160:A:MET:HE3	4	0.13
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	9	0.13
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	9	0.13
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	9	0.13
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	4	0.13
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	4	0.13
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	4	0.13
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	4	0.13
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	4	0.13
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	4	0.13
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	4	0.13
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	4	0.13
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	4	0.13
(1,516)	1:99:A:GLU:HB2	1:103:A:LEU:HG	1	0.13
(1,516)	1:99:A:GLU:HB3	1:103:A:LEU:HG	1	0.13
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB2	2	0.13
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB3	2	0.13
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB2	2	0.13
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB3	2	0.13
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE1	7	0.13
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE2	7	0.13
(1,400)	1:138:A:VAL:HB	1:160:A:MET:HE3	7	0.13
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG21	6	0.13
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG22	6	0.13
(1,386)	1:41:A:ASP:HB2	1:88:A:VAL:HG23	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	8	0.13
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	8	0.13
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	8	0.13
(1,295)	1:137:A:THR:HG21	1:160:A:MET:HA	8	0.13
(1,295)	1:137:A:THR:HG22	1:160:A:MET:HA	8	0.13
(1,295)	1:137:A:THR:HG23	1:160:A:MET:HA	8	0.13
(1,226)	1:86:A:THR:HG21	1:165:A:GLN:HA	5	0.13
(1,226)	1:86:A:THR:HG22	1:165:A:GLN:HA	5	0.13
(1,226)	1:86:A:THR:HG23	1:165:A:GLN:HA	5	0.13
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG21	6	0.12
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG22	6	0.12
(1,1148)	1:104:A:LYS:HB2	1:106:A:THR:HG23	6	0.12
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG21	6	0.12
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG22	6	0.12
(1,1148)	1:104:A:LYS:HB3	1:106:A:THR:HG23	6	0.12
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	8	0.12
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	8	0.12
(1,1097)	1:93:A:VAL:HG11	1:134:A:MET:HE1	5	0.12
(1,1097)	1:93:A:VAL:HG11	1:134:A:MET:HE2	5	0.12
(1,1097)	1:93:A:VAL:HG11	1:134:A:MET:HE3	5	0.12
(1,1097)	1:93:A:VAL:HG12	1:134:A:MET:HE1	5	0.12
(1,1097)	1:93:A:VAL:HG12	1:134:A:MET:HE2	5	0.12
(1,1097)	1:93:A:VAL:HG12	1:134:A:MET:HE3	5	0.12
(1,1097)	1:93:A:VAL:HG13	1:134:A:MET:HE1	5	0.12
(1,1097)	1:93:A:VAL:HG13	1:134:A:MET:HE2	5	0.12
(1,1097)	1:93:A:VAL:HG13	1:134:A:MET:HE3	5	0.12
(1,1097)	1:93:A:VAL:HG21	1:134:A:MET:HE1	5	0.12
(1,1097)	1:93:A:VAL:HG21	1:134:A:MET:HE2	5	0.12
(1,1097)	1:93:A:VAL:HG21	1:134:A:MET:HE3	5	0.12
(1,1097)	1:93:A:VAL:HG22	1:134:A:MET:HE1	5	0.12
(1,1097)	1:93:A:VAL:HG22	1:134:A:MET:HE2	5	0.12
(1,1097)	1:93:A:VAL:HG22	1:134:A:MET:HE3	5	0.12
(1,1097)	1:93:A:VAL:HG23	1:134:A:MET:HE1	5	0.12
(1,1097)	1:93:A:VAL:HG23	1:134:A:MET:HE2	5	0.12
(1,1097)	1:93:A:VAL:HG23	1:134:A:MET:HE3	5	0.12
(1,1059)	1:83:A:VAL:HG11	1:169:A:THR:HA	8	0.12
(1,1059)	1:83:A:VAL:HG12	1:169:A:THR:HA	8	0.12
(1,1059)	1:83:A:VAL:HG13	1:169:A:THR:HA	8	0.12
(1,1059)	1:83:A:VAL:HG21	1:169:A:THR:HA	8	0.12
(1,1059)	1:83:A:VAL:HG22	1:169:A:THR:HA	8	0.12
(1,1059)	1:83:A:VAL:HG23	1:169:A:THR:HA	8	0.12
(1,1059)	1:83:A:VAL:HG11	1:169:A:THR:HA	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:83:A:VAL:HG12	1:169:A:THR:HA	9	0.12
(1,1059)	1:83:A:VAL:HG13	1:169:A:THR:HA	9	0.12
(1,1059)	1:83:A:VAL:HG21	1:169:A:THR:HA	9	0.12
(1,1059)	1:83:A:VAL:HG22	1:169:A:THR:HA	9	0.12
(1,1059)	1:83:A:VAL:HG23	1:169:A:THR:HA	9	0.12
(1,1046)	1:80:A:GLU:HB2	1:83:A:VAL:HB	3	0.12
(1,1046)	1:80:A:GLU:HB3	1:83:A:VAL:HB	3	0.12
(1,1018)	1:71:A:GLY:HA2	1:175:A:LEU:HB2	1	0.12
(1,1018)	1:71:A:GLY:HA2	1:175:A:LEU:HB3	1	0.12
(1,1018)	1:71:A:GLY:HA3	1:175:A:LEU:HB2	1	0.12
(1,1018)	1:71:A:GLY:HA3	1:175:A:LEU:HB3	1	0.12
(1,1007)	1:67:A:LYS:HB2	1:79:A:LEU:HD11	2	0.12
(1,1007)	1:67:A:LYS:HB2	1:79:A:LEU:HD12	2	0.12
(1,1007)	1:67:A:LYS:HB2	1:79:A:LEU:HD13	2	0.12
(1,1007)	1:67:A:LYS:HB2	1:79:A:LEU:HD21	2	0.12
(1,1007)	1:67:A:LYS:HB2	1:79:A:LEU:HD22	2	0.12
(1,1007)	1:67:A:LYS:HB2	1:79:A:LEU:HD23	2	0.12
(1,1007)	1:67:A:LYS:HB3	1:79:A:LEU:HD11	2	0.12
(1,1007)	1:67:A:LYS:HB3	1:79:A:LEU:HD12	2	0.12
(1,1007)	1:67:A:LYS:HB3	1:79:A:LEU:HD13	2	0.12
(1,1007)	1:67:A:LYS:HB3	1:79:A:LEU:HD21	2	0.12
(1,1007)	1:67:A:LYS:HB3	1:79:A:LEU:HD22	2	0.12
(1,1007)	1:67:A:LYS:HB3	1:79:A:LEU:HD23	2	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD11	10	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD12	10	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD13	10	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD21	10	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD22	10	0.12
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD23	10	0.12
(1,826)	1:112:A:PHE:HD1	1:115:A:MET:HE1	9	0.12
(1,826)	1:112:A:PHE:HD1	1:115:A:MET:HE2	9	0.12
(1,826)	1:112:A:PHE:HD1	1:115:A:MET:HE3	9	0.12
(1,826)	1:112:A:PHE:HD2	1:115:A:MET:HE1	9	0.12
(1,826)	1:112:A:PHE:HD2	1:115:A:MET:HE2	9	0.12
(1,826)	1:112:A:PHE:HD2	1:115:A:MET:HE3	9	0.12
(1,729)	1:53:A:ALA:HB1	1:58:A:VAL:HG11	4	0.12
(1,729)	1:53:A:ALA:HB1	1:58:A:VAL:HG12	4	0.12
(1,729)	1:53:A:ALA:HB1	1:58:A:VAL:HG13	4	0.12
(1,729)	1:53:A:ALA:HB2	1:58:A:VAL:HG11	4	0.12
(1,729)	1:53:A:ALA:HB2	1:58:A:VAL:HG12	4	0.12
(1,729)	1:53:A:ALA:HB2	1:58:A:VAL:HG13	4	0.12
(1,729)	1:53:A:ALA:HB3	1:58:A:VAL:HG11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:53:A:ALA:HB3	1:58:A:VAL:HG12	4	0.12
(1,729)	1:53:A:ALA:HB3	1:58:A:VAL:HG13	4	0.12
(1,612)	1:121:A:GLU:HA	1:124:A:LYS:HG3	10	0.12
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB1	5	0.12
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB2	5	0.12
(1,552)	1:103:A:LEU:HG	1:150:A:ALA:HB3	5	0.12
(1,545)	1:131:A:ILE:HB	1:134:A:MET:HE1	2	0.12
(1,545)	1:131:A:ILE:HB	1:134:A:MET:HE2	2	0.12
(1,545)	1:131:A:ILE:HB	1:134:A:MET:HE3	2	0.12
(1,433)	1:115:A:MET:HE1	1:118:A:LEU:HB2	10	0.12
(1,433)	1:115:A:MET:HE2	1:118:A:LEU:HB2	10	0.12
(1,433)	1:115:A:MET:HE3	1:118:A:LEU:HB2	10	0.12
(1,313)	1:42:A:ILE:HG21	1:126:A:LEU:HA	9	0.12
(1,313)	1:42:A:ILE:HG22	1:126:A:LEU:HA	9	0.12
(1,313)	1:42:A:ILE:HG23	1:126:A:LEU:HA	9	0.12
(1,304)	1:119:A:MET:HE1	1:164:A:LEU:HA	9	0.12
(1,304)	1:119:A:MET:HE2	1:164:A:LEU:HA	9	0.12
(1,304)	1:119:A:MET:HE3	1:164:A:LEU:HA	9	0.12
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE1	2	0.12
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE2	2	0.12
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE3	2	0.12
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE1	10	0.12
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE2	10	0.12
(1,246)	1:116:A:TYR:HA	1:160:A:MET:HE3	10	0.12
(1,24)	1:150:A:ALA:H	1:153:A:VAL:H	10	0.12
(1,1248)	1:153:A:VAL:HG11	1:156:A:ILE:HG21	10	0.11
(1,1248)	1:153:A:VAL:HG11	1:156:A:ILE:HG22	10	0.11
(1,1248)	1:153:A:VAL:HG11	1:156:A:ILE:HG23	10	0.11
(1,1248)	1:153:A:VAL:HG12	1:156:A:ILE:HG21	10	0.11
(1,1248)	1:153:A:VAL:HG12	1:156:A:ILE:HG22	10	0.11
(1,1248)	1:153:A:VAL:HG12	1:156:A:ILE:HG23	10	0.11
(1,1248)	1:153:A:VAL:HG13	1:156:A:ILE:HG21	10	0.11
(1,1248)	1:153:A:VAL:HG13	1:156:A:ILE:HG22	10	0.11
(1,1248)	1:153:A:VAL:HG13	1:156:A:ILE:HG23	10	0.11
(1,1248)	1:153:A:VAL:HG21	1:156:A:ILE:HG21	10	0.11
(1,1248)	1:153:A:VAL:HG21	1:156:A:ILE:HG22	10	0.11
(1,1248)	1:153:A:VAL:HG21	1:156:A:ILE:HG23	10	0.11
(1,1248)	1:153:A:VAL:HG22	1:156:A:ILE:HG21	10	0.11
(1,1248)	1:153:A:VAL:HG22	1:156:A:ILE:HG22	10	0.11
(1,1248)	1:153:A:VAL:HG22	1:156:A:ILE:HG23	10	0.11
(1,1248)	1:153:A:VAL:HG23	1:156:A:ILE:HG21	10	0.11
(1,1248)	1:153:A:VAL:HG23	1:156:A:ILE:HG22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:153:A:VAL:HG23	1:156:A:ILE:HG23	10	0.11
(1,1127)	1:100:A:ALA:HA	1:154:A:LEU:HD11	7	0.11
(1,1127)	1:100:A:ALA:HA	1:154:A:LEU:HD12	7	0.11
(1,1127)	1:100:A:ALA:HA	1:154:A:LEU:HD13	7	0.11
(1,1127)	1:100:A:ALA:HA	1:154:A:LEU:HD21	7	0.11
(1,1127)	1:100:A:ALA:HA	1:154:A:LEU:HD22	7	0.11
(1,1127)	1:100:A:ALA:HA	1:154:A:LEU:HD23	7	0.11
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB2	5	0.11
(1,1110)	1:94:A:ILE:HB	1:161:A:ARG:HB3	5	0.11
(1,1108)	1:93:A:VAL:HG11	1:164:A:LEU:HA	6	0.11
(1,1108)	1:93:A:VAL:HG12	1:164:A:LEU:HA	6	0.11
(1,1108)	1:93:A:VAL:HG13	1:164:A:LEU:HA	6	0.11
(1,1108)	1:93:A:VAL:HG21	1:164:A:LEU:HA	6	0.11
(1,1108)	1:93:A:VAL:HG22	1:164:A:LEU:HA	6	0.11
(1,1108)	1:93:A:VAL:HG23	1:164:A:LEU:HA	6	0.11
(1,1074)	1:88:A:VAL:HG11	1:91:A:LYS:HG2	9	0.11
(1,1074)	1:88:A:VAL:HG12	1:91:A:LYS:HG2	9	0.11
(1,1074)	1:88:A:VAL:HG13	1:91:A:LYS:HG2	9	0.11
(1,1074)	1:88:A:VAL:HG21	1:91:A:LYS:HG2	9	0.11
(1,1074)	1:88:A:VAL:HG22	1:91:A:LYS:HG2	9	0.11
(1,1074)	1:88:A:VAL:HG23	1:91:A:LYS:HG2	9	0.11
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG11	8	0.11
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG12	8	0.11
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG13	8	0.11
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG21	8	0.11
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG22	8	0.11
(1,1065)	1:85:A:ALA:HB1	1:88:A:VAL:HG23	8	0.11
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG11	8	0.11
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG12	8	0.11
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG13	8	0.11
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG21	8	0.11
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG22	8	0.11
(1,1065)	1:85:A:ALA:HB2	1:88:A:VAL:HG23	8	0.11
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG11	8	0.11
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG12	8	0.11
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG13	8	0.11
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG21	8	0.11
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG22	8	0.11
(1,1065)	1:85:A:ALA:HB3	1:88:A:VAL:HG23	8	0.11
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD11	6	0.11
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD12	6	0.11
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD13	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD21	6	0.11
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD22	6	0.11
(1,949)	1:43:A:THR:HA	1:126:A:LEU:HD23	6	0.11
(1,883)	1:26:A:GLY:HA2	1:32:A:LYS:HB2	9	0.11
(1,883)	1:26:A:GLY:HA2	1:32:A:LYS:HB3	9	0.11
(1,883)	1:26:A:GLY:HA3	1:32:A:LYS:HB2	9	0.11
(1,883)	1:26:A:GLY:HA3	1:32:A:LYS:HB3	9	0.11
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE1	10	0.11
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE2	10	0.11
(1,872)	1:157:A:ALA:H	1:160:A:MET:HE3	10	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG21	8	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG22	8	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG23	8	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG21	8	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG22	8	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG23	8	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG21	9	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG22	9	0.11
(1,821)	1:112:A:PHE:HD1	1:149:A:THR:HG23	9	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG21	9	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG22	9	0.11
(1,821)	1:112:A:PHE:HD2	1:149:A:THR:HG23	9	0.11
(1,753)	1:60:A:PHE:HZ	1:129:A:LEU:H	2	0.11
(1,662)	1:46:A:ILE:HG21	1:89:A:ALA:HB1	9	0.11
(1,662)	1:46:A:ILE:HG21	1:89:A:ALA:HB2	9	0.11
(1,662)	1:46:A:ILE:HG21	1:89:A:ALA:HB3	9	0.11
(1,662)	1:46:A:ILE:HG22	1:89:A:ALA:HB1	9	0.11
(1,662)	1:46:A:ILE:HG22	1:89:A:ALA:HB2	9	0.11
(1,662)	1:46:A:ILE:HG22	1:89:A:ALA:HB3	9	0.11
(1,662)	1:46:A:ILE:HG23	1:89:A:ALA:HB1	9	0.11
(1,662)	1:46:A:ILE:HG23	1:89:A:ALA:HB2	9	0.11
(1,662)	1:46:A:ILE:HG23	1:89:A:ALA:HB3	9	0.11
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD11	5	0.11
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD12	5	0.11
(1,646)	1:82:A:LYS:HD2	1:131:A:ILE:HD13	5	0.11
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD11	5	0.11
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD12	5	0.11
(1,646)	1:82:A:LYS:HD3	1:131:A:ILE:HD13	5	0.11
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB1	2	0.11
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB2	2	0.11
(1,606)	1:49:A:ILE:HG21	1:85:A:ALA:HB3	2	0.11
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB1	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB2	2	0.11
(1,606)	1:49:A:ILE:HG22	1:85:A:ALA:HB3	2	0.11
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB1	2	0.11
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB2	2	0.11
(1,606)	1:49:A:ILE:HG23	1:85:A:ALA:HB3	2	0.11
(1,599)	1:157:A:ALA:HB1	1:160:A:MET:HA	7	0.11
(1,599)	1:157:A:ALA:HB2	1:160:A:MET:HA	7	0.11
(1,599)	1:157:A:ALA:HB3	1:160:A:MET:HA	7	0.11
(1,595)	1:82:A:LYS:HG2	1:131:A:ILE:HA	3	0.11
(1,595)	1:82:A:LYS:HG3	1:131:A:ILE:HA	3	0.11
(1,595)	1:82:A:LYS:HG2	1:131:A:ILE:HA	8	0.11
(1,595)	1:82:A:LYS:HG3	1:131:A:ILE:HA	8	0.11
(1,561)	1:42:A:ILE:HG21	1:125:A:PRO:HB3	8	0.11
(1,561)	1:42:A:ILE:HG22	1:125:A:PRO:HB3	8	0.11
(1,561)	1:42:A:ILE:HG23	1:125:A:PRO:HB3	8	0.11
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE1	8	0.11
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE2	8	0.11
(1,547)	1:118:A:LEU:HB3	1:160:A:MET:HE3	8	0.11
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB2	9	0.11
(1,514)	1:76:A:PRO:HB2	1:175:A:LEU:HB3	9	0.11
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB2	9	0.11
(1,514)	1:76:A:PRO:HB3	1:175:A:LEU:HB3	9	0.11
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB1	3	0.11
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB2	3	0.11
(1,486)	1:115:A:MET:HE1	1:150:A:ALA:HB3	3	0.11
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB1	3	0.11
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB2	3	0.11
(1,486)	1:115:A:MET:HE2	1:150:A:ALA:HB3	3	0.11
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB1	3	0.11
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB2	3	0.11
(1,486)	1:115:A:MET:HE3	1:150:A:ALA:HB3	3	0.11
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB2	9	0.11
(1,479)	1:141:A:ALA:HB1	1:155:A:GLU:HB3	9	0.11
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB2	9	0.11
(1,479)	1:141:A:ALA:HB2	1:155:A:GLU:HB3	9	0.11
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB2	9	0.11
(1,479)	1:141:A:ALA:HB3	1:155:A:GLU:HB3	9	0.11
(1,473)	1:134:A:MET:HE1	1:163:A:LYS:HD2	4	0.11
(1,473)	1:134:A:MET:HE2	1:163:A:LYS:HD2	4	0.11
(1,473)	1:134:A:MET:HE3	1:163:A:LYS:HD2	4	0.11
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE1	7	0.11
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:96:A:ILE:HA	1:160:A:MET:HE3	7	0.11
(1,360)	1:53:A:ALA:HA	1:58:A:VAL:HB	8	0.11
(1,348)	1:39:A:ALA:HB1	1:122:A:VAL:HA	1	0.11
(1,348)	1:39:A:ALA:HB2	1:122:A:VAL:HA	1	0.11
(1,348)	1:39:A:ALA:HB3	1:122:A:VAL:HA	1	0.11
(1,322)	1:96:A:ILE:HD11	1:115:A:MET:HA	6	0.11
(1,322)	1:96:A:ILE:HD12	1:115:A:MET:HA	6	0.11
(1,322)	1:96:A:ILE:HD13	1:115:A:MET:HA	6	0.11
(1,231)	1:27:A:LEU:HA	1:31:A:THR:HG21	6	0.11
(1,231)	1:27:A:LEU:HA	1:31:A:THR:HG22	6	0.11
(1,231)	1:27:A:LEU:HA	1:31:A:THR:HG23	6	0.11
(1,226)	1:86:A:THR:HG21	1:165:A:GLN:HA	10	0.11
(1,226)	1:86:A:THR:HG22	1:165:A:GLN:HA	10	0.11
(1,226)	1:86:A:THR:HG23	1:165:A:GLN:HA	10	0.11
(1,1276)	1:172:A:TYR:HB2	1:176:A:LYS:HG2	4	0.1
(1,1276)	1:172:A:TYR:HB2	1:176:A:LYS:HG3	4	0.1
(1,1276)	1:172:A:TYR:HB3	1:176:A:LYS:HG2	4	0.1
(1,1276)	1:172:A:TYR:HB3	1:176:A:LYS:HG3	4	0.1
(1,1169)	1:116:A:TYR:HD1	1:153:A:VAL:HG11	1	0.1
(1,1169)	1:116:A:TYR:HD1	1:153:A:VAL:HG12	1	0.1
(1,1169)	1:116:A:TYR:HD1	1:153:A:VAL:HG13	1	0.1
(1,1169)	1:116:A:TYR:HD1	1:153:A:VAL:HG21	1	0.1
(1,1169)	1:116:A:TYR:HD1	1:153:A:VAL:HG22	1	0.1
(1,1169)	1:116:A:TYR:HD1	1:153:A:VAL:HG23	1	0.1
(1,1169)	1:116:A:TYR:HD2	1:153:A:VAL:HG11	1	0.1
(1,1169)	1:116:A:TYR:HD2	1:153:A:VAL:HG12	1	0.1
(1,1169)	1:116:A:TYR:HD2	1:153:A:VAL:HG13	1	0.1
(1,1169)	1:116:A:TYR:HD2	1:153:A:VAL:HG21	1	0.1
(1,1169)	1:116:A:TYR:HD2	1:153:A:VAL:HG22	1	0.1
(1,1169)	1:116:A:TYR:HD2	1:153:A:VAL:HG23	1	0.1
(1,1059)	1:83:A:VAL:HG11	1:169:A:THR:HA	1	0.1
(1,1059)	1:83:A:VAL:HG12	1:169:A:THR:HA	1	0.1
(1,1059)	1:83:A:VAL:HG13	1:169:A:THR:HA	1	0.1
(1,1059)	1:83:A:VAL:HG21	1:169:A:THR:HA	1	0.1
(1,1059)	1:83:A:VAL:HG22	1:169:A:THR:HA	1	0.1
(1,1059)	1:83:A:VAL:HG23	1:169:A:THR:HA	1	0.1
(1,719)	1:42:A:ILE:HD11	1:89:A:ALA:HB1	2	0.1
(1,719)	1:42:A:ILE:HD11	1:89:A:ALA:HB2	2	0.1
(1,719)	1:42:A:ILE:HD11	1:89:A:ALA:HB3	2	0.1
(1,719)	1:42:A:ILE:HD12	1:89:A:ALA:HB1	2	0.1
(1,719)	1:42:A:ILE:HD12	1:89:A:ALA:HB2	2	0.1
(1,719)	1:42:A:ILE:HD12	1:89:A:ALA:HB3	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:42:A:ILE:HD13	1:89:A:ALA:HB1	2	0.1
(1,719)	1:42:A:ILE:HD13	1:89:A:ALA:HB2	2	0.1
(1,719)	1:42:A:ILE:HD13	1:89:A:ALA:HB3	2	0.1
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG11	2	0.1
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG12	2	0.1
(1,711)	1:46:A:ILE:HD11	1:88:A:VAL:HG13	2	0.1
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG11	2	0.1
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG12	2	0.1
(1,711)	1:46:A:ILE:HD12	1:88:A:VAL:HG13	2	0.1
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG11	2	0.1
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG12	2	0.1
(1,711)	1:46:A:ILE:HD13	1:88:A:VAL:HG13	2	0.1
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG21	6	0.1
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG22	6	0.1
(1,664)	1:60:A:PHE:HA	1:78:A:ILE:HG23	6	0.1
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB1	1	0.1
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB2	1	0.1
(1,615)	1:53:A:ALA:HB1	1:81:A:ALA:HB3	1	0.1
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB1	1	0.1
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB2	1	0.1
(1,615)	1:53:A:ALA:HB2	1:81:A:ALA:HB3	1	0.1
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB1	1	0.1
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB2	1	0.1
(1,615)	1:53:A:ALA:HB3	1:81:A:ALA:HB3	1	0.1
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB1	6	0.1
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB2	6	0.1
(1,590)	1:31:A:THR:HG21	1:95:A:ALA:HB3	6	0.1
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB1	6	0.1
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB2	6	0.1
(1,590)	1:31:A:THR:HG22	1:95:A:ALA:HB3	6	0.1
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB1	6	0.1
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB2	6	0.1
(1,590)	1:31:A:THR:HG23	1:95:A:ALA:HB3	6	0.1
(1,551)	1:150:A:ALA:HB1	1:154:A:LEU:HG	1	0.1
(1,551)	1:150:A:ALA:HB2	1:154:A:LEU:HG	1	0.1
(1,551)	1:150:A:ALA:HB3	1:154:A:LEU:HG	1	0.1
(1,492)	1:147:A:PRO:HG2	1:156:A:ILE:HG21	9	0.1
(1,492)	1:147:A:PRO:HG2	1:156:A:ILE:HG22	9	0.1
(1,492)	1:147:A:PRO:HG2	1:156:A:ILE:HG23	9	0.1

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

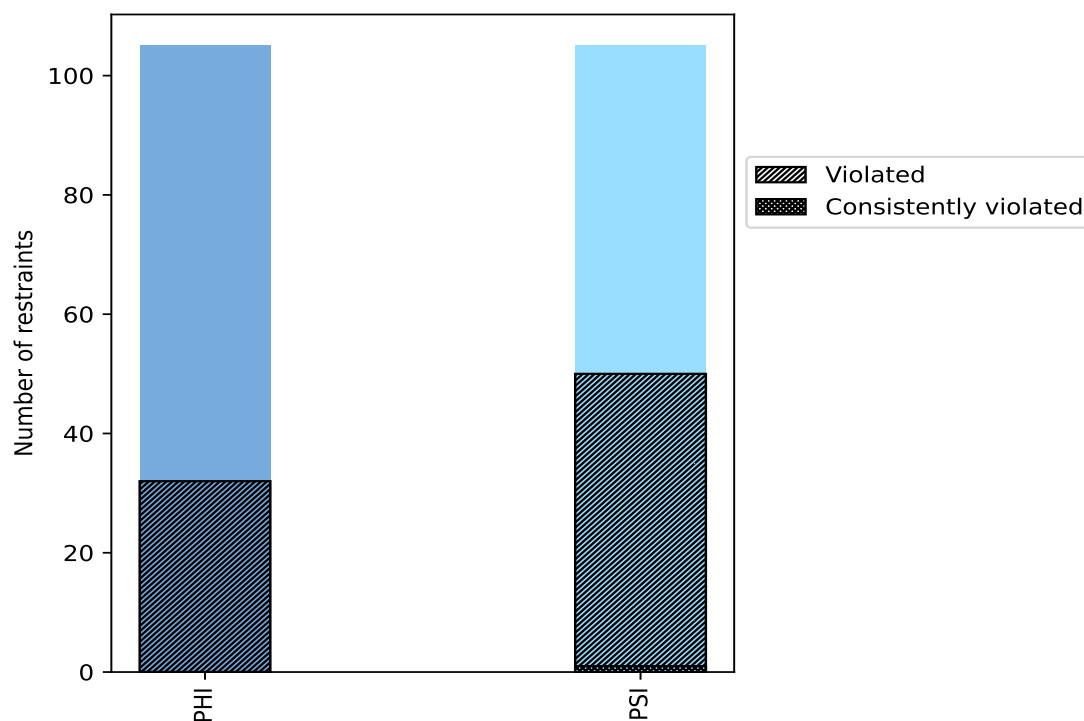
### 10.1 Summary of dihedral-angle violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	105	50.0	32	30.5	15.2	0	0.0	0.0
PSI	105	50.0	50	47.6	23.8	1	1.0	0.5
Total	210	100.0	82	39.0	39.0	1	0.5	0.5

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

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



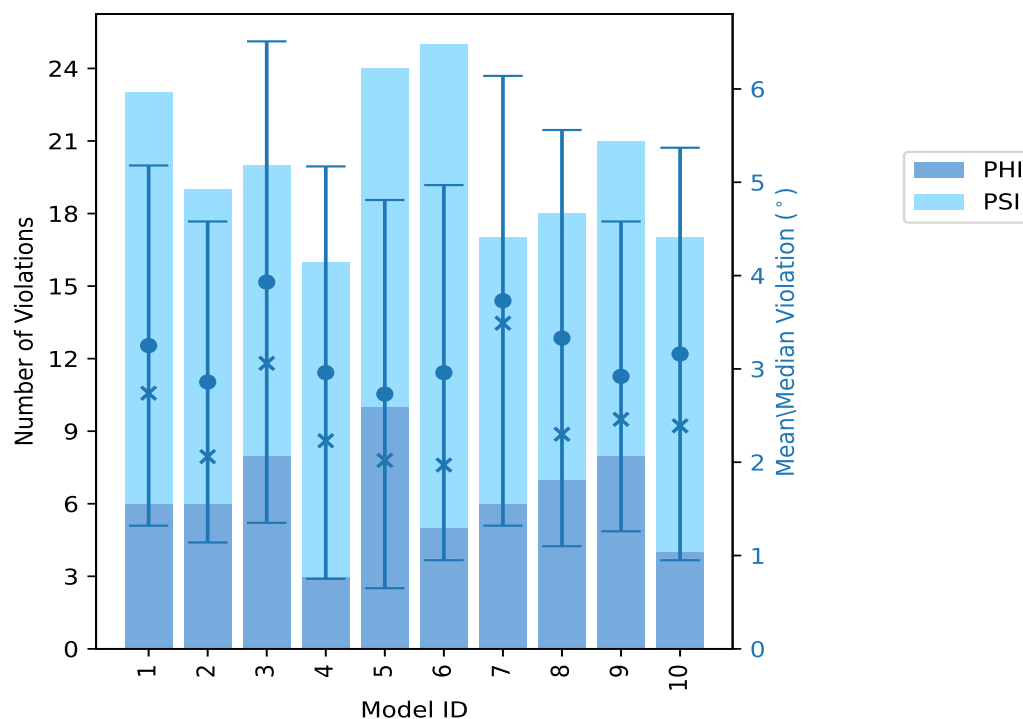
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	6	17	23	3.25	8.56	1.93	2.74
2	6	13	19	2.86	7.04	1.72	2.06
3	8	12	20	3.93	10.44	2.58	3.06
4	3	13	16	2.96	8.54	2.21	2.23
5	10	14	24	2.73	10.85	2.08	2.02
6	5	20	25	2.96	8.82	2.01	1.97
7	6	11	17	3.73	9.76	2.41	3.49
8	7	11	18	3.33	9.38	2.23	2.3
9	8	13	21	2.92	6.97	1.66	2.46
10	4	13	17	3.16	8.31	2.21	2.39

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



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

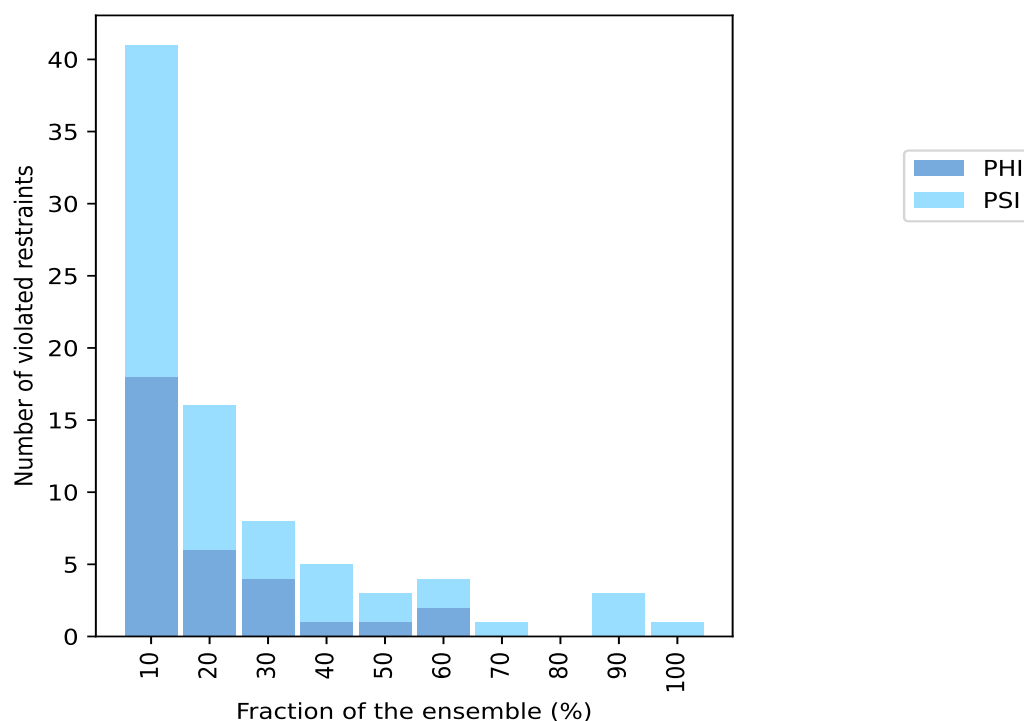
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
18	23	41	1	10.0
6	10	16	2	20.0
4	4	8	3	30.0
1	4	5	4	40.0
1	2	3	5	50.0
2	2	4	6	60.0
0	1	1	7	70.0
0	0	0	8	80.0
0	3	3	9	90.0
0	1	1	10	100.0

<sup>1</sup> Number of models with violations

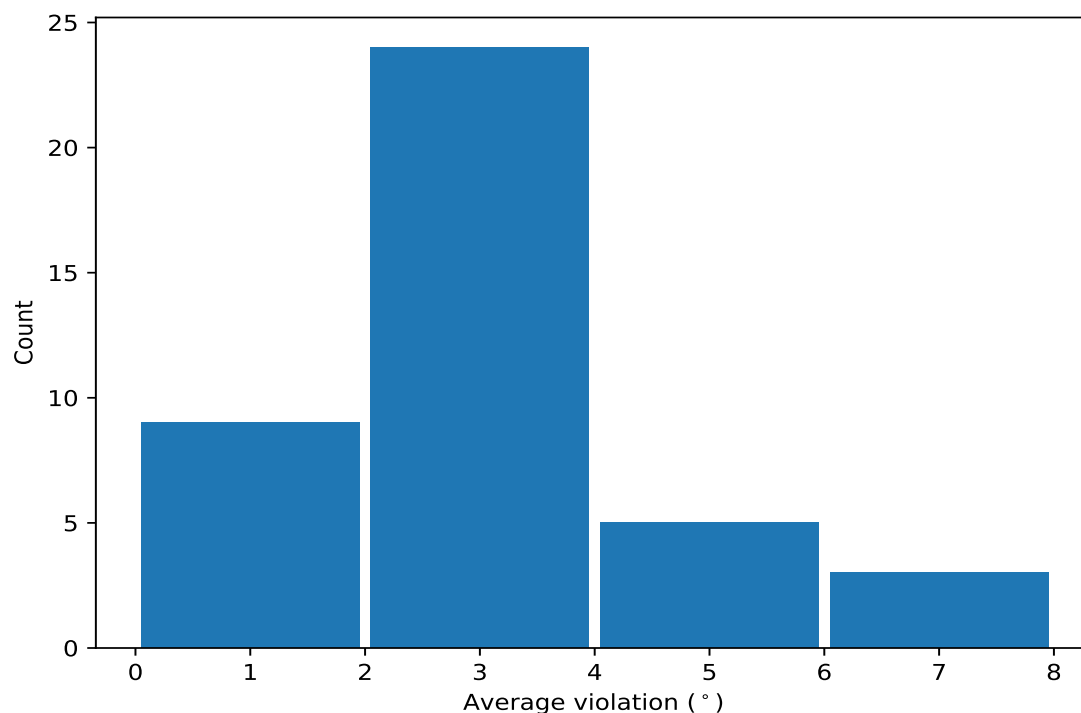
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	10	6.66	1.28	6.52
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	9	6.9	2.59	6.72
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	9	4.08	1.52	3.95
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	9	3.55	0.76	3.48
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	7	2.54	1.24	1.82
(1,56)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:ALA:N	6	4.12	1.98	3.84
(1,110)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:MET:N	6	2.98	1.81	2.36
(1,25)	1:42:A:ILE:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	6	2.02	0.46	2.02
(1,35)	1:47:A:ASP:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	6	1.93	0.52	1.91
(1,71)	1:87:A:THR:C	1:88:A:VAL:N	1:88:A:VAL:CA	1:88:A:VAL:C	5	5.08	3.38	3.13
(1,128)	1:123:A:SER:N	1:123:A:SER:CA	1:123:A:SER:C	1:124:A:LYS:N	5	3.67	2.06	3.02
(1,172)	1:160:A:MET:N	1:160:A:MET:CA	1:160:A:MET:C	1:161:A:ARG:N	5	3.38	1.55	2.93
(1,132)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:GLN:N	4	4.3	1.36	4.61

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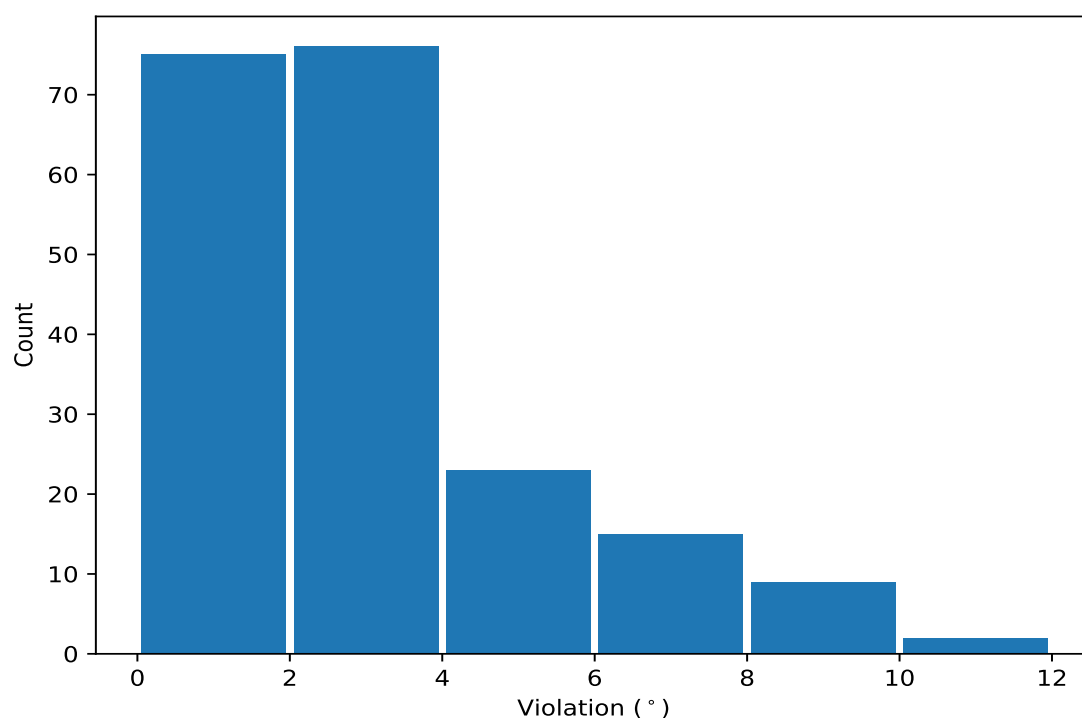
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,210)	1:179:A:GLU:N	1:179:A:GLU:CA	1:179:A:GLU:C	1:180:A:ASN:N	4	3.51	2.22	2.99
(1,152)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:ALA:N	4	2.52	0.67	2.56
(1,144)	1:137:A:THR:N	1:137:A:THR:CA	1:137:A:THR:C	1:138:A:VAL:N	4	2.25	1.22	2.24
(1,187)	1:167:A:VAL:C	1:168:A:HIS:N	1:168:A:HIS:CA	1:168:A:HIS:C	4	1.59	0.29	1.56
(1,141)	1:135:A:THR:C	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	3	5.47	3.05	6.54
(1,139)	1:134:A:MET:C	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	3	3.33	2.34	2.22
(1,111)	1:114:A:ALA:C	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	3	2.93	0.79	2.68
(1,174)	1:161:A:ARG:N	1:161:A:ARG:CA	1:161:A:ARG:C	1:162:A:GLU:N	3	2.93	0.84	3.25
(1,114)	1:116:A:TYR:N	1:116:A:TYR:CA	1:116:A:TYR:C	1:117:A:ASP:N	3	2.78	1.52	2.15
(1,163)	1:155:A:GLU:C	1:156:A:ILE:N	1:156:A:ILE:CA	1:156:A:ILE:C	3	2.7	1.09	3.06
(1,18)	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	1:40:A:LYS:N	3	1.57	0.08	1.54
(1,70)	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	1:88:A:VAL:N	3	1.25	0.19	1.21
(1,58)	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	1:82:A:LYS:N	2	6.0	4.44	6.0
(1,115)	1:116:A:TYR:C	1:117:A:ASP:N	1:117:A:ASP:CA	1:117:A:ASP:C	2	3.84	0.42	3.84
(1,36)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:ILE:N	2	3.16	0.66	3.16
(1,135)	1:127:A:GLN:C	1:128:A:LYS:N	1:128:A:LYS:CA	1:128:A:LYS:C	2	3.08	1.66	3.08
(1,142)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:THR:N	2	3.05	0.0	3.05
(1,180)	1:164:A:LEU:N	1:164:A:LEU:CA	1:164:A:LEU:C	1:165:A:GLN:N	2	2.53	0.14	2.53
(1,81)	1:92:A:PHE:C	1:93:A:VAL:N	1:93:A:VAL:CA	1:93:A:VAL:C	2	2.34	0.26	2.34
(1,46)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:ALA:N	2	2.3	0.31	2.3
(1,49)	1:76:A:PRO:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	2	2.24	0.28	2.24
(1,162)	1:153:A:VAL:N	1:153:A:VAL:CA	1:153:A:VAL:C	1:154:A:LEU:N	2	2.15	0.16	2.15
(1,112)	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	1:116:A:TYR:N	2	2.1	0.56	2.1
(1,38)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:LYS:N	2	1.77	0.05	1.77
(1,137)	1:133:A:GLU:C	1:134:A:MET:N	1:134:A:MET:CA	1:134:A:MET:C	2	1.76	0.03	1.76
(1,136)	1:128:A:LYS:N	1:128:A:LYS:CA	1:128:A:LYS:C	1:129:A:LEU:N	2	1.55	0.18	1.55
(1,125)	1:121:A:GLU:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	2	1.44	0.02	1.44
(1,202)	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	1:176:A:LYS:N	2	1.16	0.14	1.16

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	5	10.85
(1,58)	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	1:82:A:LYS:N	3	10.44
(1,71)	1:87:A:THR:C	1:88:A:VAL:N	1:88:A:VAL:CA	1:88:A:VAL:C	7	9.76
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	8	9.38
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	6	8.82
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	3	8.6
(1,141)	1:135:A:THR:C	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1	8.56
(1,71)	1:87:A:THR:C	1:88:A:VAL:N	1:88:A:VAL:CA	1:88:A:VAL:C	4	8.54
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	10	8.31
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	4	8.29
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	3	8.19
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	10	7.86
(1,56)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:ALA:N	7	7.21
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	2	7.04
(1,210)	1:179:A:GLU:N	1:179:A:GLU:CA	1:179:A:GLU:C	1:180:A:ASN:N	9	6.97
(1,128)	1:123:A:SER:N	1:123:A:SER:CA	1:123:A:SER:C	1:124:A:LYS:N	10	6.92
(1,110)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:MET:N	3	6.92
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	6	6.8
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	9	6.72
(1,139)	1:134:A:MET:C	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1	6.58
(1,141)	1:135:A:THR:C	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	2	6.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,172)	1:160:A:MET:N	1:160:A:MET:CA	1:160:A:MET:C	1:161:A:ARG:N	8	6.4
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	7	6.34
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	7	6.25
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	8	6.25
(1,17)	1:38:A:SER:C	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	6	6.16
(1,56)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:ALA:N	8	5.83
(1,132)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:GLN:N	5	5.8
(1,153)	1:141:A:ALA:C	1:142:A:ALA:N	1:142:A:ALA:CA	1:142:A:ALA:C	3	5.71
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	9	5.68
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	1	5.55
(1,132)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:GLN:N	1	5.08
(1,128)	1:123:A:SER:N	1:123:A:SER:CA	1:123:A:SER:C	1:124:A:LYS:N	1	5.0
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	1	4.95
(1,114)	1:116:A:TYR:N	1:116:A:TYR:CA	1:116:A:TYR:C	1:117:A:ASP:N	7	4.87
(1,56)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:ALA:N	6	4.81
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	2	4.76
(1,135)	1:127:A:GLN:C	1:128:A:LYS:N	1:128:A:LYS:CA	1:128:A:LYS:C	6	4.73
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	6	4.67
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	5	4.4
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	7	4.29
(1,115)	1:116:A:TYR:C	1:117:A:ASP:N	1:117:A:ASP:CA	1:117:A:ASP:C	8	4.25
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	2	4.22
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	1	4.21
(1,130)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:PRO:N	5	4.2
(1,132)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:GLN:N	3	4.14
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	9	4.13
(1,177)	1:162:A:GLU:C	1:163:A:LYS:N	1:163:A:LYS:CA	1:163:A:LYS:C	2	4.11
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	1	4.06
(1,111)	1:114:A:ALA:C	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	5	3.99
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	4	3.95
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	7	3.94
(1,210)	1:179:A:GLU:N	1:179:A:GLU:CA	1:179:A:GLU:C	1:180:A:ASN:N	6	3.85
(1,163)	1:155:A:GLU:C	1:156:A:ILE:N	1:156:A:ILE:CA	1:156:A:ILE:C	7	3.82
(1,36)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:ILE:N	8	3.82
(1,1)	1:30:A:ALA:C	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	3	3.8
(1,174)	1:161:A:ARG:N	1:161:A:ARG:CA	1:161:A:ARG:C	1:162:A:GLU:N	6	3.76
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	2	3.74
(1,101)	1:109:A:SER:C	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	5	3.52
(1,144)	1:137:A:THR:N	1:137:A:THR:CA	1:137:A:THR:C	1:138:A:VAL:N	7	3.49
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	3	3.49
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	8	3.48
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	1	3.45
(1,144)	1:137:A:THR:N	1:137:A:THR:CA	1:137:A:THR:C	1:138:A:VAL:N	9	3.44
(1,121)	1:119:A:MET:C	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	10	3.42
(1,115)	1:116:A:TYR:C	1:117:A:ASP:N	1:117:A:ASP:CA	1:117:A:ASP:C	9	3.42
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	4	3.4
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	6	3.38
(1,134)	1:127:A:GLN:N	1:127:A:GLN:CA	1:127:A:GLN:C	1:128:A:LYS:N	10	3.29
(1,152)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:ALA:N	3	3.28
(1,174)	1:161:A:ARG:N	1:161:A:ARG:CA	1:161:A:ARG:C	1:162:A:GLU:N	9	3.25
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	8	3.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	1:54:A:ALA:N	1:54:A:ALA:CA	1:54:A:ALA:C	1:55:A:LEU:N	5	3.21
(1,71)	1:87:A:THR:C	1:88:A:VAL:N	1:88:A:VAL:CA	1:88:A:VAL:C	10	3.13
(1,152)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:ALA:N	1	3.09
(1,163)	1:155:A:GLU:C	1:156:A:ILE:N	1:156:A:ILE:CA	1:156:A:ILE:C	3	3.06
(1,172)	1:160:A:MET:N	1:160:A:MET:CA	1:160:A:MET:C	1:161:A:ARG:N	9	3.05
(1,142)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:THR:N	3	3.05
(1,142)	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	1:137:A:THR:N	4	3.05
(1,128)	1:123:A:SER:N	1:123:A:SER:CA	1:123:A:SER:C	1:124:A:LYS:N	6	3.02
(1,203)	1:175:A:LEU:C	1:176:A:LYS:N	1:176:A:LYS:CA	1:176:A:LYS:C	5	3.01
(1,172)	1:160:A:MET:N	1:160:A:MET:CA	1:160:A:MET:C	1:161:A:ARG:N	1	2.93
(1,56)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:ALA:N	3	2.87
(1,188)	1:168:A:HIS:N	1:168:A:HIS:CA	1:168:A:HIS:C	1:169:A:THR:N	1	2.74
(1,35)	1:47:A:ASP:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	2	2.72
(1,25)	1:42:A:ILE:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	9	2.71
(1,110)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:MET:N	2	2.69
(1,111)	1:114:A:ALA:C	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	3	2.68
(1,180)	1:164:A:LEU:N	1:164:A:LEU:CA	1:164:A:LEU:C	1:165:A:GLN:N	4	2.67
(1,112)	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	1:116:A:TYR:N	2	2.66
(1,46)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:ALA:N	10	2.61
(1,81)	1:92:A:PHE:C	1:93:A:VAL:N	1:93:A:VAL:CA	1:93:A:VAL:C	9	2.6
(1,110)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:MET:N	1	2.57
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	5	2.57
(1,49)	1:76:A:PRO:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	7	2.52
(1,36)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:ILE:N	10	2.5
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	5	2.47
(1,140)	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	1:136:A:LYS:N	4	2.46
(1,71)	1:87:A:THR:C	1:88:A:VAL:N	1:88:A:VAL:CA	1:88:A:VAL:C	9	2.46
(1,32)	1:46:A:ILE:N	1:46:A:ILE:CA	1:46:A:ILE:C	1:47:A:ASP:N	9	2.41
(1,180)	1:164:A:LEU:N	1:164:A:LEU:CA	1:164:A:LEU:C	1:165:A:GLN:N	10	2.39
(1,35)	1:47:A:ASP:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	8	2.34
(1,25)	1:42:A:ILE:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	1	2.34
(1,22)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:ILE:N	7	2.33
(1,176)	1:162:A:GLU:N	1:162:A:GLU:CA	1:162:A:GLU:C	1:163:A:LYS:N	6	2.31
(1,162)	1:153:A:VAL:N	1:153:A:VAL:CA	1:153:A:VAL:C	1:154:A:LEU:N	4	2.31
(1,172)	1:160:A:MET:N	1:160:A:MET:CA	1:160:A:MET:C	1:161:A:ARG:N	10	2.27
(1,128)	1:123:A:SER:N	1:123:A:SER:CA	1:123:A:SER:C	1:124:A:LYS:N	8	2.25
(1,16)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:ALA:N	3	2.24
(1,172)	1:160:A:MET:N	1:160:A:MET:CA	1:160:A:MET:C	1:161:A:ARG:N	3	2.23
(1,139)	1:134:A:MET:C	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	9	2.22
(1,132)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:GLN:N	6	2.18
(1,114)	1:116:A:TYR:N	1:116:A:TYR:CA	1:116:A:TYR:C	1:117:A:ASP:N	4	2.15
(1,110)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:MET:N	8	2.15
(1,210)	1:179:A:GLU:N	1:179:A:GLU:CA	1:179:A:GLU:C	1:180:A:ASN:N	8	2.12
(1,111)	1:114:A:ALA:C	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	9	2.11
(1,110)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:MET:N	9	2.11
(1,81)	1:92:A:PHE:C	1:93:A:VAL:N	1:93:A:VAL:CA	1:93:A:VAL:C	5	2.08
(1,56)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:ALA:N	2	2.06
(1,35)	1:47:A:ASP:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	4	2.04
(1,152)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:ALA:N	5	2.03
(1,68)	1:86:A:THR:N	1:86:A:THR:CA	1:86:A:THR:C	1:87:A:THR:N	1	2.03
(1,25)	1:42:A:ILE:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	3	2.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,187)	1:167:A:VAL:C	1:168:A:HIS:N	1:168:A:HIS:CA	1:168:A:HIS:C	5	2.01
(1,25)	1:42:A:ILE:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	2	2.01
(1,162)	1:153:A:VAL:N	1:153:A:VAL:CA	1:153:A:VAL:C	1:154:A:LEU:N	2	1.99
(1,46)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:ALA:N	1	1.98
(1,64)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:ALA:N	6	1.97
(1,49)	1:76:A:PRO:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	6	1.96
(1,56)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:ALA:N	4	1.94
(1,113)	1:115:A:MET:C	1:116:A:TYR:N	1:116:A:TYR:CA	1:116:A:TYR:C	6	1.85
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	10	1.82
(1,38)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:LYS:N	6	1.82
(1,137)	1:133:A:GLU:C	1:134:A:MET:N	1:134:A:MET:CA	1:134:A:MET:C	2	1.79
(1,35)	1:47:A:ASP:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	7	1.78
(1,25)	1:42:A:ILE:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	5	1.78
(1,174)	1:161:A:ARG:N	1:161:A:ARG:CA	1:161:A:ARG:C	1:162:A:GLU:N	2	1.77
(1,12)	1:36:A:GLU:N	1:36:A:GLU:CA	1:36:A:GLU:C	1:37:A:ARG:N	10	1.76
(1,137)	1:133:A:GLU:C	1:134:A:MET:N	1:134:A:MET:CA	1:134:A:MET:C	6	1.73
(1,136)	1:128:A:LYS:N	1:128:A:LYS:CA	1:128:A:LYS:C	1:129:A:LEU:N	1	1.73
(1,201)	1:174:A:THR:C	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	10	1.72
(1,38)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:LYS:N	10	1.72
(1,120)	1:119:A:MET:N	1:119:A:MET:CA	1:119:A:MET:C	1:120:A:PHE:N	10	1.71
(1,152)	1:141:A:ALA:N	1:141:A:ALA:CA	1:141:A:ALA:C	1:142:A:ALA:N	4	1.7
(1,18)	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	1:40:A:LYS:N	5	1.69
(1,187)	1:167:A:VAL:C	1:168:A:HIS:N	1:168:A:HIS:CA	1:168:A:HIS:C	8	1.68
(1,78)	1:91:A:LYS:N	1:91:A:LYS:CA	1:91:A:LYS:C	1:92:A:PHE:N	5	1.63
(1,35)	1:47:A:ASP:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	9	1.59
(1,58)	1:81:A:ALA:N	1:81:A:ALA:CA	1:81:A:ALA:C	1:82:A:LYS:N	7	1.56
(1,21)	1:40:A:LYS:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	3	1.56
(1,165)	1:156:A:ILE:C	1:157:A:ALA:N	1:157:A:ALA:CA	1:157:A:ALA:C	5	1.54
(1,112)	1:115:A:MET:N	1:115:A:MET:CA	1:115:A:MET:C	1:116:A:TYR:N	9	1.54
(1,18)	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	1:40:A:LYS:N	3	1.54
(1,71)	1:87:A:THR:C	1:88:A:VAL:N	1:88:A:VAL:CA	1:88:A:VAL:C	2	1.51
(1,178)	1:163:A:LYS:N	1:163:A:LYS:CA	1:163:A:LYS:C	1:164:A:LEU:N	8	1.5
(1,70)	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	1:88:A:VAL:N	7	1.5
(1,18)	1:39:A:ALA:N	1:39:A:ALA:CA	1:39:A:ALA:C	1:40:A:LYS:N	9	1.49
(1,158)	1:151:A:GLN:N	1:151:A:GLN:CA	1:151:A:GLN:C	1:152:A:GLY:N	1	1.48
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	2	1.47
(1,2)	1:31:A:THR:N	1:31:A:THR:CA	1:31:A:THR:C	1:32:A:LYS:N	6	1.47
(1,119)	1:118:A:LEU:C	1:119:A:MET:N	1:119:A:MET:CA	1:119:A:MET:C	3	1.46
(1,125)	1:121:A:GLU:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	7	1.45
(1,85)	1:94:A:ILE:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	5	1.45
(1,187)	1:167:A:VAL:C	1:168:A:HIS:N	1:168:A:HIS:CA	1:168:A:HIS:C	9	1.44
(1,109)	1:113:A:SER:C	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	8	1.44
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	4	1.42
(1,135)	1:127:A:GLN:C	1:128:A:LYS:N	1:128:A:LYS:CA	1:128:A:LYS:C	1	1.42
(1,125)	1:121:A:GLU:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	5	1.42
(1,110)	1:114:A:ALA:N	1:114:A:ALA:CA	1:114:A:ALA:C	1:115:A:MET:N	6	1.42
(1,136)	1:128:A:LYS:N	1:128:A:LYS:CA	1:128:A:LYS:C	1:129:A:LEU:N	6	1.37
(1,20)	1:40:A:LYS:N	1:40:A:LYS:CA	1:40:A:LYS:C	1:41:A:ASP:N	5	1.36
(1,184)	1:166:A:ARG:N	1:166:A:ARG:CA	1:166:A:ARG:C	1:167:A:VAL:N	1	1.33
(1,67)	1:85:A:ALA:C	1:86:A:THR:N	1:86:A:THR:CA	1:86:A:THR:C	3	1.33
(1,141)	1:135:A:THR:C	1:136:A:LYS:N	1:136:A:LYS:CA	1:136:A:LYS:C	8	1.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,114)	1:116:A:TYR:N	1:116:A:TYR:CA	1:116:A:TYR:C	1:117:A:ASP:N	5	1.31
(1,202)	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	1:176:A:LYS:N	1	1.29
(1,84)	1:94:A:ILE:N	1:94:A:ILE:CA	1:94:A:ILE:C	1:95:A:ALA:N	6	1.29
(1,150)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:ALA:N	6	1.27
(1,25)	1:42:A:ILE:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	8	1.24
(1,207)	1:177:A:LYS:C	1:178:A:LYS:N	1:178:A:LYS:CA	1:178:A:LYS:C	10	1.23
(1,187)	1:167:A:VAL:C	1:168:A:HIS:N	1:168:A:HIS:CA	1:168:A:HIS:C	4	1.23
(1,163)	1:155:A:GLU:C	1:156:A:ILE:N	1:156:A:ILE:CA	1:156:A:ILE:C	8	1.23
(1,3)	1:31:A:THR:C	1:32:A:LYS:N	1:32:A:LYS:CA	1:32:A:LYS:C	5	1.23
(1,70)	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	1:88:A:VAL:N	2	1.21
(1,8)	1:34:A:ARG:N	1:34:A:ARG:CA	1:34:A:ARG:C	1:35:A:LEU:N	6	1.21
(1,179)	1:163:A:LYS:C	1:164:A:LEU:N	1:164:A:LEU:CA	1:164:A:LEU:C	1	1.19
(1,139)	1:134:A:MET:C	1:135:A:THR:N	1:135:A:THR:CA	1:135:A:THR:C	7	1.19
(1,128)	1:123:A:SER:N	1:123:A:SER:CA	1:123:A:SER:C	1:124:A:LYS:N	4	1.15
(1,194)	1:171:A:ASN:N	1:171:A:ASN:CA	1:171:A:ASN:C	1:172:A:TYR:N	2	1.12
(1,210)	1:179:A:GLU:N	1:179:A:GLU:CA	1:179:A:GLU:C	1:180:A:ASN:N	7	1.11
(1,35)	1:47:A:ASP:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1	1.1
(1,154)	1:142:A:ALA:N	1:142:A:ALA:CA	1:142:A:ALA:C	1:143:A:GLU:N	6	1.09
(1,144)	1:137:A:THR:N	1:137:A:THR:CA	1:137:A:THR:C	1:138:A:VAL:N	5	1.05
(1,70)	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	1:88:A:VAL:N	10	1.03
(1,202)	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	1:176:A:LYS:N	4	1.02
(1,86)	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	1:96:A:ILE:N	9	1.02
(1,50)	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	1:78:A:ILE:N	2	1.02
(1,144)	1:137:A:THR:N	1:137:A:THR:CA	1:137:A:THR:C	1:138:A:VAL:N	6	1.01
(1,24)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:THR:N	9	1.01
(1,10)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:GLU:N	5	1.01