



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 02:32 AM UTC

PDB ID : 2MTC / pdb\_00002mtc  
BMRB ID : 25156  
Title : Structure of decorin binding protein A from strain N40 of Borrelia burgdorferi  
Authors : Wang, X.; Morgan, A.  
Deposited on : 2014-08-16

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

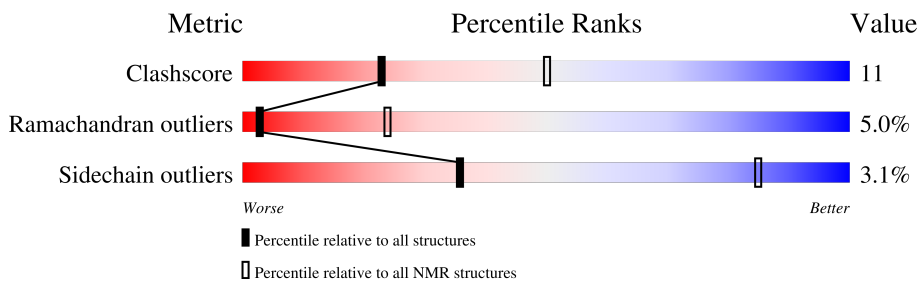
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 56%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	166	75% 17% • 5%

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:68, (158)	A:76-A:194 1.08	6

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2587 atoms, of which 1310 are hydrogens and 0 are deuteriums.

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

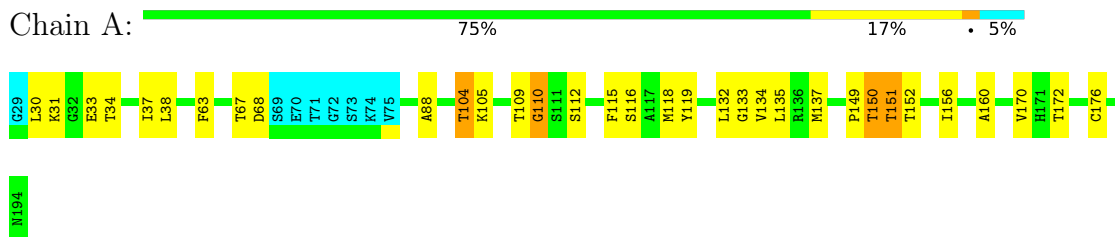
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	166	2587	794	1310	217	259	7	0

## 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

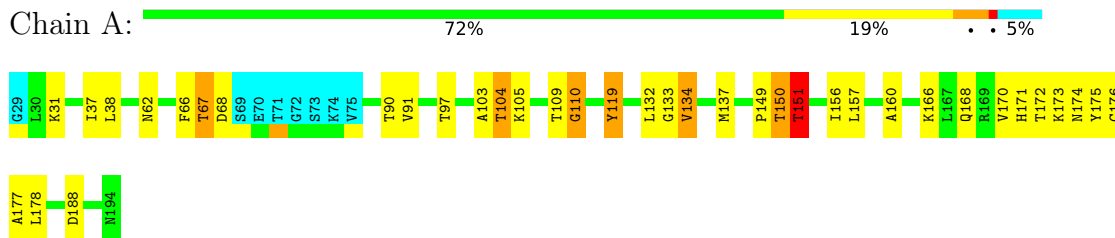


### 4.2 Scores per residue for each member of the ensemble

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

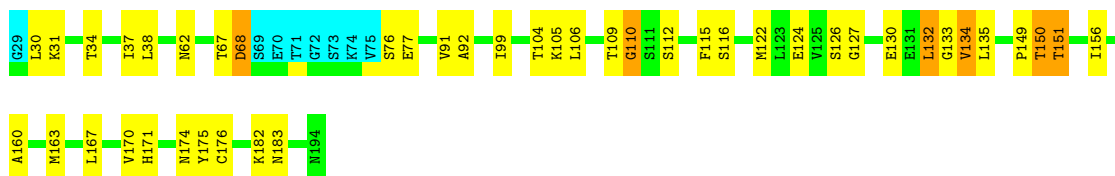




### 4.2.3 Score per residue for model 3

- Molecule 1: Decorin-binding protein A

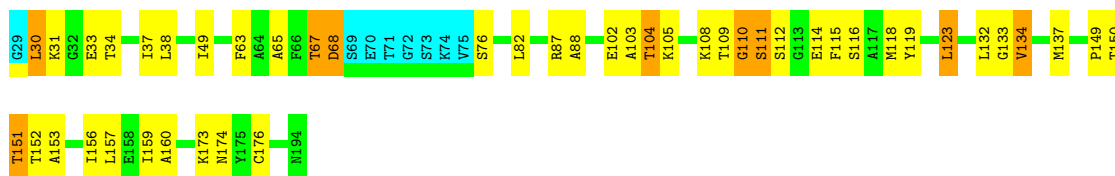
Chain A: 69% 23% 5%



### 4.2.4 Score per residue for model 4

- Molecule 1: Decorin-binding protein A

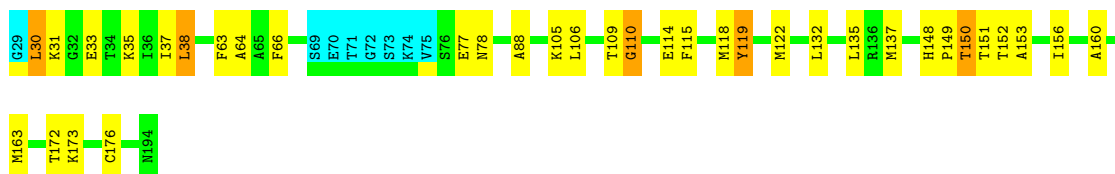
Chain A: 67% 22% 5% 5%



### 4.2.5 Score per residue for model 5

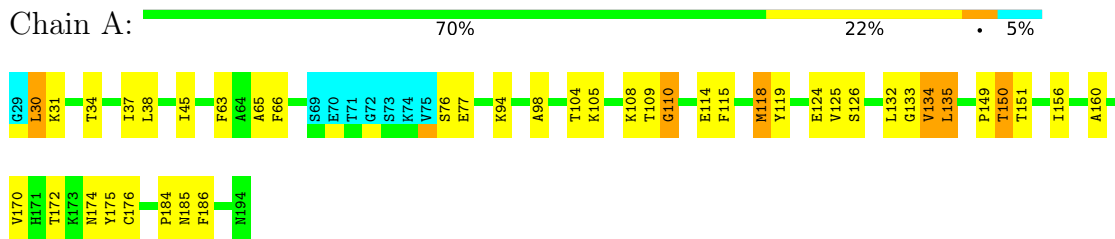
- Molecule 1: Decorin-binding protein A

Chain A: 73% 19% 5%



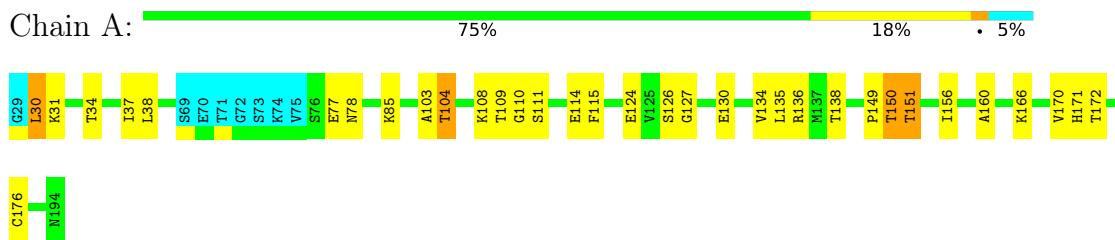
### 4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Decorin-binding protein A



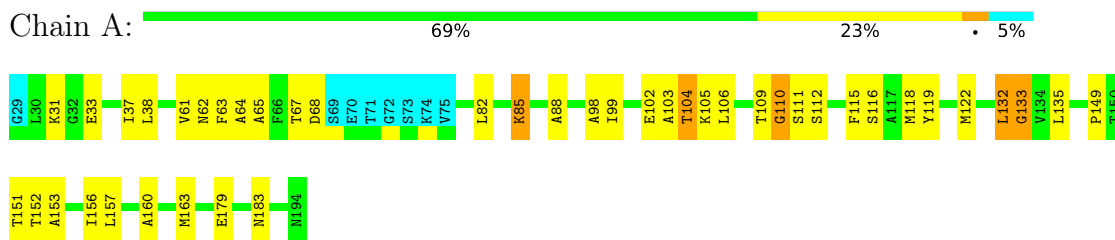
#### 4.2.7 Score per residue for model 7

- Molecule 1: Decorin-binding protein A



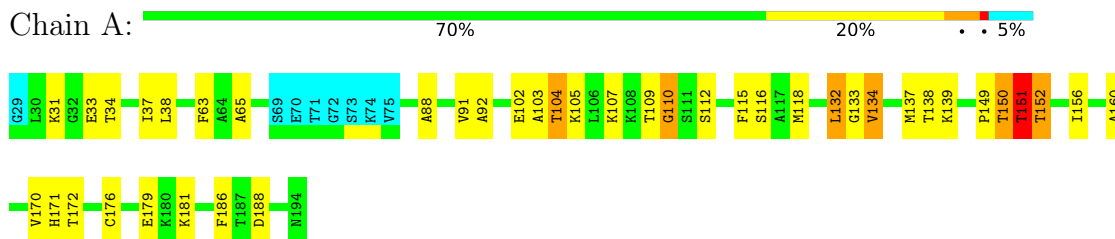
#### 4.2.8 Score per residue for model 8

- Molecule 1: Decorin-binding protein A



#### 4.2.9 Score per residue for model 9

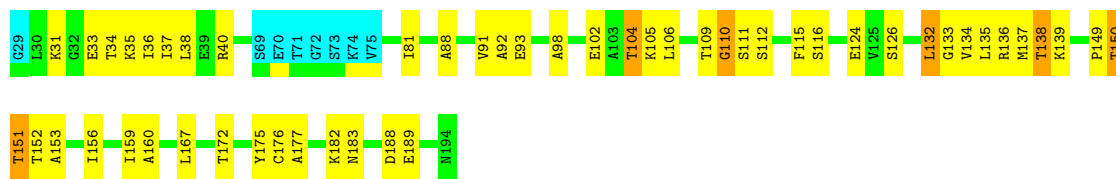
- Molecule 1: Decorin-binding protein A



#### 4.2.10 Score per residue for model 10

- Molecule 1: Decorin-binding protein A

Chain A:  64% 27% 5%



## 5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure solution	
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	1246
Number of shifts mapped to atoms	1246
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	56%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.64±0.01	0±0/1237 ( 0.0± 0.0%)	0.91±0.01	0±0/1658 ( 0.0± 0.0%)
All	All	0.64	0/12370 ( 0.0%)	0.91	1/16580 ( 0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	148	HIS	CA-CB-CG	-5.04	108.76	113.80	5	1

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1225	1257	1255	28±5
All	All	12250	12570	12550	278

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:150:THR:O	1:A:151:THR:HG23	0.69	1.88	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:PHE:CD1	1:A:116:SER:N	0.62	2.68	2	6
1:A:132:LEU:O	1:A:132:LEU:HD23	0.61	1.95	5	2
1:A:119:TYR:CB	1:A:151:THR:HG21	0.61	2.25	1	1
1:A:88:ALA:HB2	1:A:132:LEU:HD13	0.61	1.71	10	5
1:A:156:ILE:O	1:A:160:ALA:HB2	0.59	1.97	3	10
1:A:33:GLU:H	1:A:33:GLU:CD	0.58	2.06	4	1
1:A:81:ILE:N	1:A:81:ILE:HD12	0.58	2.14	10	1
1:A:149:PRO:O	1:A:150:THR:C	0.57	2.48	7	5
1:A:104:THR:HG23	1:A:105:LYS:N	0.56	2.15	4	1
1:A:104:THR:HG23	1:A:105:LYS:H	0.55	1.61	4	1
1:A:134:VAL:O	1:A:134:VAL:HG13	0.54	2.02	6	1
1:A:63:PHE:CE1	1:A:66:PHE:CE2	0.53	2.96	5	1
1:A:135:LEU:HD12	1:A:135:LEU:N	0.53	2.19	8	5
1:A:167:LEU:O	1:A:167:LEU:HD23	0.52	2.04	10	1
1:A:112:SER:O	1:A:115:PHE:CE2	0.52	2.63	8	3
1:A:170:VAL:HG13	1:A:171:HIS:N	0.52	2.20	7	3
1:A:122:MET:SD	1:A:163:MET:SD	0.51	3.08	8	2
1:A:149:PRO:O	1:A:151:THR:N	0.51	2.44	2	5
1:A:109:THR:OG1	1:A:115:PHE:CE2	0.50	2.64	7	1
1:A:103:ALA:O	1:A:104:THR:O	0.50	2.29	9	2
1:A:174:ASN:OD1	1:A:175:TYR:N	0.50	2.44	6	4
1:A:108:LYS:N	1:A:108:LYS:CD	0.50	2.75	4	3
1:A:37:ILE:HG23	1:A:38:LEU:N	0.49	2.22	3	10
1:A:64:ALA:O	1:A:68:ASP:N	0.49	2.45	8	1
1:A:149:PRO:O	1:A:159:ILE:HD11	0.49	2.08	10	3
1:A:109:THR:O	1:A:110:GLY:C	0.49	2.56	3	6
1:A:173:LYS:O	1:A:176:CYS:SG	0.49	2.71	1	3
1:A:170:VAL:O	1:A:174:ASN:ND2	0.49	2.46	6	3
1:A:82:LEU:HD12	1:A:82:LEU:N	0.49	2.21	4	2
1:A:61:VAL:O	1:A:63:PHE:N	0.49	2.46	8	1
1:A:88:ALA:HB2	1:A:132:LEU:HD23	0.49	1.85	4	1
1:A:137:MET:C	1:A:139:LYS:N	0.49	2.71	10	3
1:A:110:GLY:N	1:A:114:GLU:OE1	0.49	2.45	5	4
1:A:85:LYS:NZ	1:A:133:GLY:O	0.49	2.45	8	1
1:A:119:TYR:C	1:A:119:TYR:CD1	0.49	2.91	8	2
1:A:66:PHE:CD1	1:A:132:LEU:O	0.48	2.66	1	2
1:A:78:ASN:OD1	1:A:79:SER:N	0.48	2.47	2	1
1:A:98:ALA:O	1:A:102:GLU:N	0.48	2.44	10	2
1:A:109:THR:O	1:A:111:SER:N	0.48	2.46	10	2
1:A:135:LEU:N	1:A:135:LEU:CD1	0.48	2.77	7	4
1:A:188:ASP:OD1	1:A:189:GLU:N	0.47	2.48	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:O	1:A:37:ILE:N	0.47	2.46	8	3
1:A:152:THR:OG1	1:A:153:ALA:N	0.47	2.48	8	1
1:A:119:TYR:HB2	1:A:151:THR:HG21	0.47	1.87	1	1
1:A:157:LEU:HD22	1:A:157:LEU:N	0.47	2.25	1	1
1:A:137:MET:O	1:A:137:MET:SD	0.46	2.73	10	2
1:A:91:VAL:HG13	1:A:92:ALA:N	0.46	2.24	3	2
1:A:99:ILE:CD1	1:A:122:MET:CE	0.46	2.93	8	1
1:A:184:PRO:C	1:A:186:PHE:H	0.46	2.18	6	2
1:A:30:LEU:HD12	1:A:30:LEU:N	0.46	2.26	4	3
1:A:122:MET:HE1	1:A:163:MET:SD	0.46	2.50	3	1
1:A:179:GLU:OE1	1:A:186:PHE:CE1	0.46	2.68	9	1
1:A:63:PHE:C	1:A:65:ALA:N	0.46	2.73	8	5
1:A:179:GLU:CD	1:A:186:PHE:CE1	0.46	2.93	9	1
1:A:137:MET:O	1:A:139:LYS:N	0.46	2.48	10	1
1:A:174:ASN:C	1:A:176:CYS:N	0.46	2.72	3	3
1:A:82:LEU:N	1:A:82:LEU:CD1	0.46	2.79	4	2
1:A:172:THR:O	1:A:176:CYS:SG	0.46	2.73	7	5
1:A:151:THR:O	1:A:156:ILE:N	0.46	2.49	9	1
1:A:166:LYS:O	1:A:170:VAL:HG12	0.45	2.11	7	2
1:A:127:GLY:O	1:A:130:GLU:N	0.45	2.49	7	2
1:A:182:LYS:CD	1:A:182:LYS:N	0.45	2.78	3	1
1:A:104:THR:OG1	1:A:105:LYS:N	0.45	2.50	10	3
1:A:34:THR:O	1:A:37:ILE:HG22	0.45	2.12	3	5
1:A:119:TYR:CZ	1:A:123:LEU:HD23	0.45	2.46	4	1
1:A:124:GLU:C	1:A:126:SER:N	0.45	2.74	6	4
1:A:104:THR:CG2	1:A:105:LYS:H	0.45	2.24	4	1
1:A:81:ILE:N	1:A:81:ILE:CD1	0.45	2.79	10	1
1:A:111:SER:OG	1:A:114:GLU:N	0.45	2.49	4	1
1:A:150:THR:O	1:A:151:THR:C	0.45	2.60	2	2
1:A:114:GLU:O	1:A:118:MET:SD	0.45	2.75	5	1
1:A:125:VAL:HG12	1:A:125:VAL:O	0.45	2.12	6	1
1:A:112:SER:O	1:A:115:PHE:CD1	0.44	2.70	2	3
1:A:45:ILE:HD12	1:A:45:ILE:N	0.44	2.27	6	1
1:A:170:VAL:HG23	1:A:171:HIS:N	0.44	2.28	3	2
1:A:37:ILE:CG2	1:A:38:LEU:N	0.44	2.80	3	8
1:A:133:GLY:O	1:A:134:VAL:O	0.44	2.36	1	4
1:A:157:LEU:N	1:A:157:LEU:CD2	0.44	2.81	1	1
1:A:170:VAL:CG1	1:A:171:HIS:N	0.44	2.80	1	3
1:A:114:GLU:O	1:A:117:ALA:N	0.44	2.50	2	1
1:A:182:LYS:C	1:A:183:ASN:ND2	0.44	2.75	10	1
1:A:102:GLU:OE1	1:A:118:MET:SD	0.44	2.76	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ILE:HG23	1:A:132:LEU:HD13	0.44	1.89	4	1
1:A:157:LEU:HD12	1:A:157:LEU:N	0.44	2.28	8	2
1:A:183:ASN:N	1:A:183:ASN:OD1	0.44	2.51	2	1
1:A:150:THR:HG22	1:A:151:THR:OG1	0.44	2.13	3	1
1:A:109:THR:OG1	1:A:115:PHE:CZ	0.44	2.69	6	1
1:A:134:VAL:HG12	1:A:135:LEU:N	0.44	2.28	10	1
1:A:136:ARG:C	1:A:138:THR:N	0.44	2.75	10	1
1:A:91:VAL:CG1	1:A:92:ALA:N	0.43	2.81	3	3
1:A:119:TYR:CD1	1:A:119:TYR:C	0.43	2.95	5	2
1:A:98:ALA:O	1:A:101:GLY:N	0.43	2.52	2	1
1:A:119:TYR:CE1	1:A:123:LEU:HD23	0.43	2.49	4	1
1:A:38:LEU:O	1:A:38:LEU:HD13	0.43	2.14	5	1
1:A:64:ALA:C	1:A:66:PHE:N	0.43	2.77	5	1
1:A:137:MET:C	1:A:137:MET:SD	0.43	3.02	9	1
1:A:134:VAL:CG1	1:A:135:LEU:N	0.43	2.81	10	1
1:A:66:PHE:CG	1:A:132:LEU:O	0.43	2.70	1	1
1:A:152:THR:O	1:A:153:ALA:C	0.43	2.62	10	4
1:A:106:LEU:O	1:A:110:GLY:N	0.43	2.52	8	2
1:A:108:LYS:O	1:A:114:GLU:CD	0.43	2.62	6	1
1:A:124:GLU:C	1:A:126:SER:H	0.43	2.21	6	2
1:A:134:VAL:HG22	1:A:135:LEU:N	0.43	2.28	7	1
1:A:102:GLU:C	1:A:104:THR:N	0.43	2.75	9	1
1:A:105:LYS:C	1:A:107:LYS:N	0.43	2.76	9	1
1:A:30:LEU:N	1:A:30:LEU:CD1	0.43	2.82	7	2
1:A:104:THR:CG2	1:A:105:LYS:N	0.42	2.80	4	1
1:A:171:HIS:O	1:A:175:TYR:N	0.42	2.48	1	1
1:A:99:ILE:CD1	1:A:122:MET:HE2	0.42	2.44	3	1
1:A:112:SER:O	1:A:115:PHE:CE1	0.42	2.73	2	2
1:A:94:LYS:O	1:A:98:ALA:N	0.42	2.49	6	1
1:A:167:LEU:HD23	1:A:167:LEU:C	0.42	2.39	10	1
1:A:102:GLU:CD	1:A:118:MET:SD	0.42	3.03	8	1
1:A:176:CYS:SG	1:A:188:ASP:OD2	0.42	2.78	9	1
1:A:63:PHE:C	1:A:65:ALA:H	0.42	2.23	2	1
1:A:33:GLU:C	1:A:35:LYS:N	0.42	2.77	10	2
1:A:90:THR:HG23	1:A:91:VAL:N	0.41	2.30	1	1
1:A:168:GLN:O	1:A:172:THR:HG22	0.41	2.14	1	1
1:A:67:THR:O	1:A:68:ASP:O	0.41	2.36	3	2
1:A:93:GLU:CD	1:A:167:LEU:HD21	0.41	2.40	10	1
1:A:175:TYR:C	1:A:177:ALA:N	0.41	2.78	10	1
1:A:156:ILE:O	1:A:160:ALA:CB	0.41	2.68	8	1
1:A:135:LEU:N	1:A:135:LEU:HD12	0.41	2.30	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:LEU:CD1	1:A:167:LEU:N	0.41	2.83	3	1
1:A:179:GLU:O	1:A:183:ASN:OD1	0.41	2.39	8	1
1:A:136:ARG:C	1:A:138:THR:H	0.41	2.22	7	1
1:A:176:CYS:SG	1:A:177:ALA:N	0.41	2.94	1	1
1:A:103:ALA:O	1:A:104:THR:C	0.41	2.64	1	3
1:A:174:ASN:O	1:A:176:CYS:N	0.41	2.54	3	1
1:A:179:GLU:CD	1:A:186:PHE:CD1	0.41	2.99	9	1
1:A:151:THR:O	1:A:152:THR:C	0.41	2.64	9	1
1:A:109:THR:O	1:A:115:PHE:CE1	0.40	2.75	5	1
1:A:36:ILE:HD12	1:A:40:ARG:HE	0.40	1.76	10	1
1:A:167:LEU:N	1:A:167:LEU:HD12	0.40	2.31	3	1
1:A:150:THR:O	1:A:151:THR:CG2	0.40	2.65	1	1
1:A:188:ASP:OD1	1:A:188:ASP:N	0.40	2.54	1	1
1:A:123:LEU:HD13	1:A:123:LEU:O	0.40	2.17	4	1
1:A:115:PHE:O	1:A:118:MET:CG	0.40	2.69	6	1
1:A:166:LYS:O	1:A:170:VAL:CG1	0.40	2.69	7	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/166 (95%)	134±2 (86±1%)	15±2 (9±2%)	8±2 (5±1%)	3	24
All	All	1570/1660 (95%)	1343 (86%)	148 (9%)	79 (5%)	3	24

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	104	THR	9
1	A	110	GLY	9
1	A	150	THR	9
1	A	134	VAL	6
1	A	105	LYS	5
1	A	62	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	68	ASP	4
1	A	76	SER	4
1	A	30	LEU	4
1	A	137	MET	3
1	A	151	THR	3
1	A	135	LEU	3
1	A	133	GLY	3
1	A	149	PRO	2
1	A	106	LEU	2
1	A	77	GLU	2
1	A	78	ASN	2
1	A	185	ASN	1
1	A	111	SER	1
1	A	152	THR	1
1	A	34	THR	1
1	A	138	THR	1

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	135/141 (96%)	131±1 (97±1%)	4±1 (3±1%)	36 85
All	All	1350/1410 (96%)	1308 (97%)	42 (3%)	36 85

All 16 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	151	THR	10
1	A	31	LYS	9
1	A	132	LEU	5
1	A	67	THR	3
1	A	119	TYR	2
1	A	38	LEU	2
1	A	87	ARG	2
1	A	97	THR	1
1	A	178	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	183	ASN	1
1	A	111	SER	1
1	A	123	LEU	1
1	A	118	MET	1
1	A	85	LYS	1
1	A	138	THR	1
1	A	181	LYS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 56% for the well-defined parts and 56% 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 [i](#)

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	1246
Number of shifts mapped to atoms	1246
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	163	$-0.37 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	152	$0.60 \pm 0.08$	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	154	$0.37 \pm 0.26$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 56%, i.e. 1196 atoms were assigned a chemical shift out of a possible 2127. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	606/791 (77%)	302/320 (94%)	156/316 (49%)	148/155 (95%)
Sidechain	590/1242 (48%)	333/802 (42%)	255/394 (65%)	2/46 (4%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/94 (0%)	0/46 (0%)	0/44 (0%)	0/4 (0%)
Overall	1196/2127 (56%)	635/1168 (54%)	411/754 (55%)	150/205 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 56%, i.e. 1246 atoms were assigned a chemical shift out of a possible 2211. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	633/833 (76%)	316/338 (93%)	163/332 (49%)	154/163 (94%)
Sidechain	613/1284 (48%)	347/829 (42%)	264/408 (65%)	2/47 (4%)
Aromatic	0/94 (0%)	0/46 (0%)	0/44 (0%)	0/4 (0%)
Overall	1246/2211 (56%)	663/1213 (55%)	427/784 (54%)	156/214 (73%)

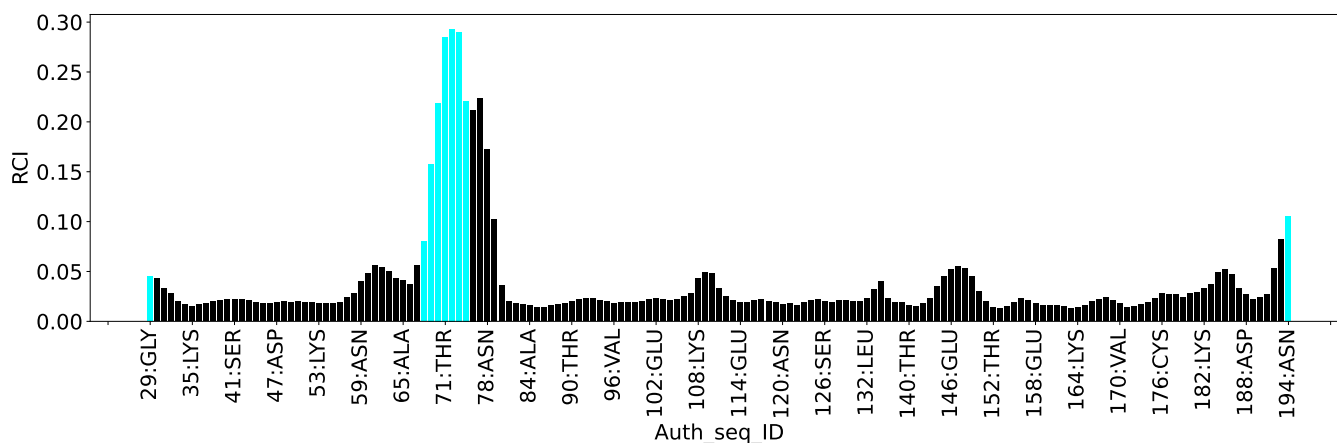
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1831
Intra-residue ( $ i-j =0$ )	401
Sequential ( $ i-j =1$ )	483
Medium range ( $ i-j >1$ and $ i-j <5$ )	433
Long range ( $ i-j \geq 5$ )	514
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	260
Number of unmapped restraints	0
Number of restraints per residue	12.6
Number of long range restraints per residue <sup>1</sup>	3.1

<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)	50.0	0.2
0.2-0.5 (Medium)	27.9	0.49
>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)	11.1	6.48
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis i

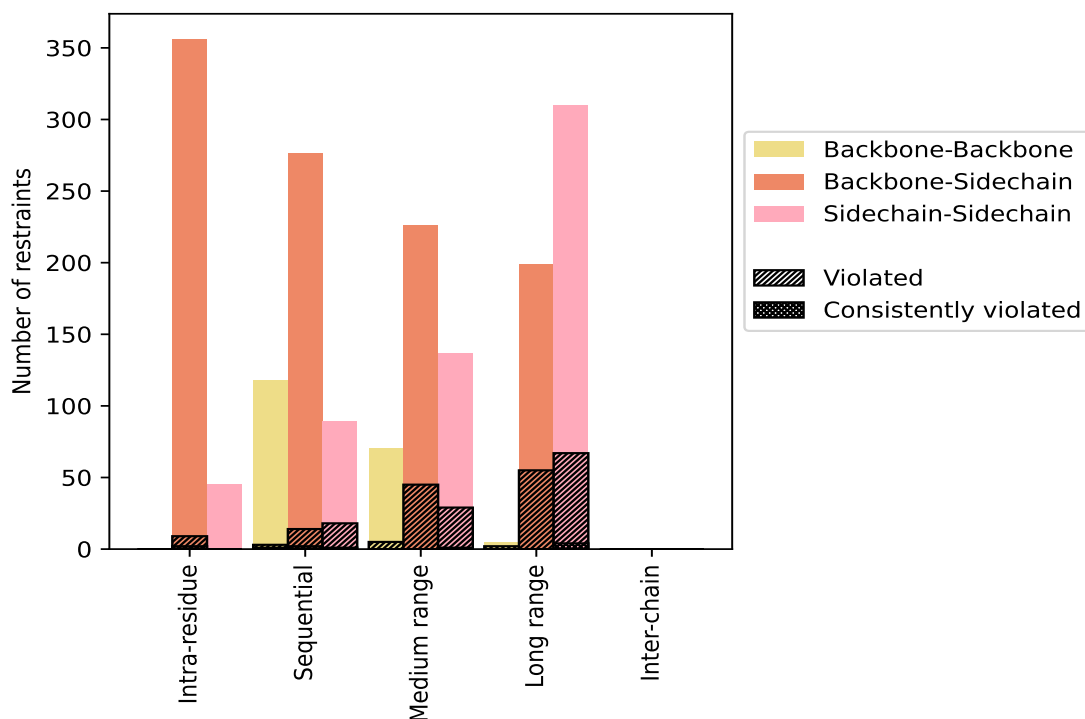
### 9.1 Summary of distance violations i

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>401</b>	<b>21.9</b>	<b>9</b>	<b>2.2</b>	<b>0.5</b>	<b>2</b>	<b>0.5</b>	<b>0.1</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	356	19.4	9	2.5	0.5	2	0.6	0.1
Sidechain-Sidechain	45	2.5	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>483</b>	<b>26.4</b>	<b>35</b>	<b>7.2</b>	<b>1.9</b>	<b>4</b>	<b>0.8</b>	<b>0.2</b>
Backbone-Backbone	118	6.4	3	2.5	0.2	1	0.8	0.1
Backbone-Sidechain	276	15.1	14	5.1	0.8	2	0.7	0.1
Sidechain-Sidechain	89	4.9	18	20.2	1.0	1	1.1	0.1
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>433</b>	<b>23.6</b>	<b>79</b>	<b>18.2</b>	<b>4.3</b>	<b>1</b>	<b>0.2</b>	<b>0.1</b>
Backbone-Backbone	70	3.8	5	7.1	0.3	0	0.0	0.0
Backbone-Sidechain	226	12.3	45	19.9	2.5	0	0.0	0.0
Sidechain-Sidechain	137	7.5	29	21.2	1.6	1	0.7	0.1
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>514</b>	<b>28.1</b>	<b>124</b>	<b>24.1</b>	<b>6.8</b>	<b>4</b>	<b>0.8</b>	<b>0.2</b>
Backbone-Backbone	5	0.3	2	40.0	0.1	0	0.0	0.0
Backbone-Sidechain	199	10.9	55	27.6	3.0	0	0.0	0.0
Sidechain-Sidechain	310	16.9	67	21.6	3.7	4	1.3	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>1831</b>	<b>100.0</b>	<b>247</b>	<b>13.5</b>	<b>13.5</b>	<b>11</b>	<b>0.6</b>	<b>0.6</b>
Backbone-Backbone	193	10.5	10	5.2	0.5	1	0.5	0.1
Backbone-Sidechain	1057	57.7	123	11.6	6.7	4	0.4	0.2
Sidechain-Sidechain	581	31.7	114	19.6	6.2	6	1.0	0.3

<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 disulfid bonds are counted in their appropriate category on the x-axis

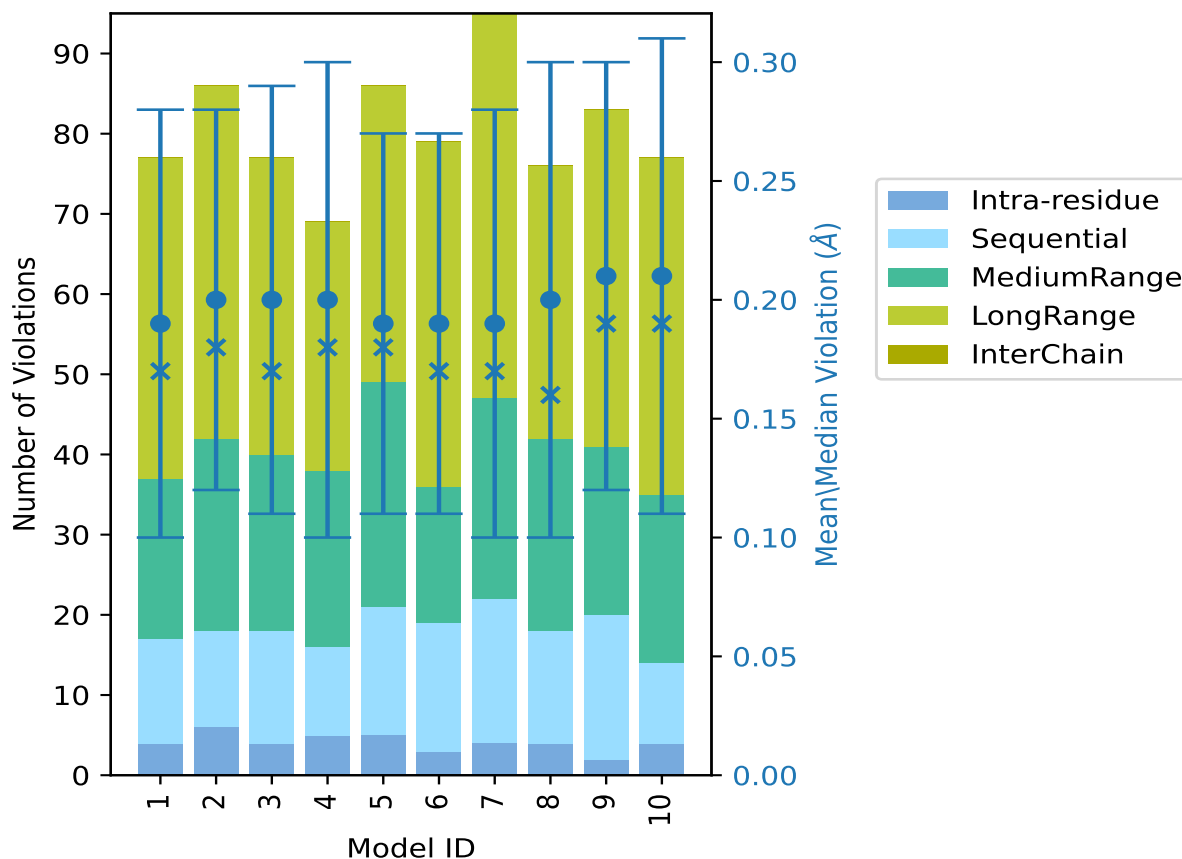
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <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	4	13	20	40	0	77	0.19	0.49	0.09	0.17
2	6	12	24	44	0	86	0.2	0.47	0.08	0.18
3	4	14	22	37	0	77	0.2	0.48	0.09	0.17
4	5	11	22	31	0	69	0.2	0.48	0.1	0.18
5	5	16	28	37	0	86	0.19	0.49	0.08	0.18
6	3	16	17	43	0	79	0.19	0.46	0.08	0.17
7	4	18	25	48	0	95	0.19	0.49	0.09	0.17
8	4	14	24	34	0	76	0.2	0.44	0.1	0.16
9	2	18	21	42	0	83	0.21	0.49	0.09	0.19
10	4	10	21	42	0	77	0.21	0.49	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, 1584(IR:392, SQ:448, MR:354, LR:390, 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>	%
3	13	34	41	0	91	1	10.0
0	5	11	23	0	39	2	20.0
1	2	11	19	0	33	3	30.0

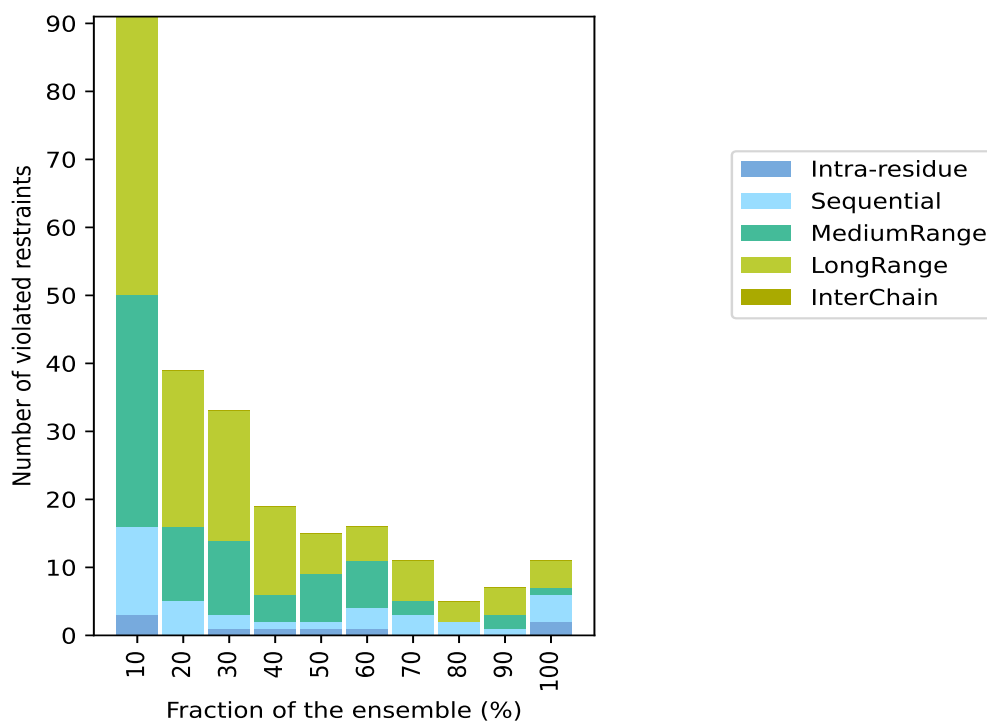
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
1	1	4	13	0	19	4	40.0
1	1	7	6	0	15	5	50.0
1	3	7	5	0	16	6	60.0
0	3	2	6	0	11	7	70.0
0	2	0	3	0	5	8	80.0
0	1	2	4	0	7	9	90.0
2	4	1	4	0	11	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](#)

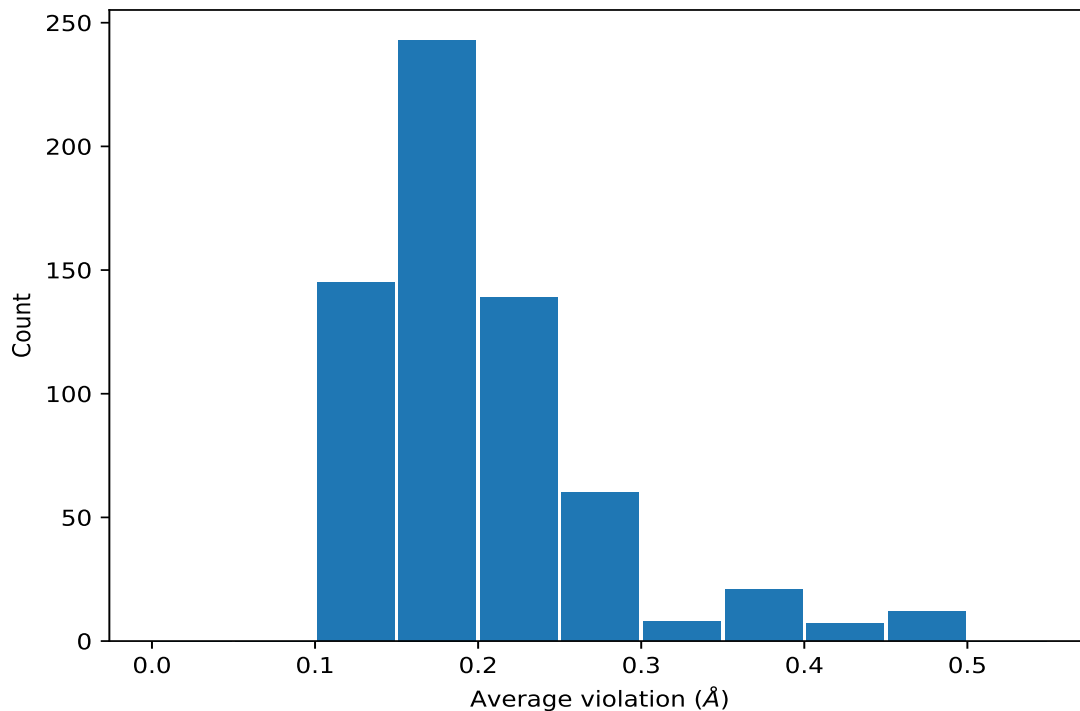


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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)
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	10	0.37	0.1	0.39
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	10	0.37	0.1	0.39
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	10	0.37	0.1	0.39
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	10	0.37	0.1	0.39
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	10	0.29	0.04	0.3
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	10	0.29	0.04	0.3
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	10	0.28	0.1	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	10	0.28	0.1	0.28
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	10	0.28	0.1	0.28
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	10	0.23	0.05	0.24
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	10	0.23	0.05	0.24
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	10	0.2	0.07	0.21
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	10	0.2	0.07	0.21
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	10	0.2	0.07	0.21
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	10	0.18	0.05	0.17
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	10	0.18	0.05	0.17
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	10	0.15	0.03	0.16
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	10	0.15	0.03	0.14
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	10	0.15	0.03	0.14
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	10	0.14	0.04	0.13
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	10	0.14	0.04	0.13
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	10	0.14	0.04	0.13
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	10	0.14	0.03	0.14
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	10	0.14	0.03	0.14
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	10	0.14	0.03	0.14
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	10	0.14	0.03	0.14
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	10	0.14	0.03	0.14
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	10	0.14	0.03	0.14
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	10	0.12	0.01	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	10	0.12	0.01	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	10	0.12	0.01	0.12
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	9	0.35	0.09	0.36
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	9	0.35	0.09	0.36
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	9	0.35	0.09	0.36
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	9	0.29	0.06	0.29
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	9	0.27	0.09	0.25
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	9	0.27	0.09	0.25
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	9	0.27	0.09	0.25
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	9	0.2	0.03	0.2
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	9	0.2	0.03	0.2
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	9	0.2	0.04	0.18
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	9	0.19	0.01	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	9	0.16	0.05	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	9	0.16	0.05	0.13
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	8	0.34	0.05	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	8	0.34	0.05	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	8	0.34	0.05	0.36
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	8	0.3	0.12	0.3
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	8	0.3	0.12	0.3
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	8	0.21	0.08	0.19
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	8	0.21	0.08	0.19
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	8	0.21	0.08	0.19
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	8	0.19	0.04	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	8	0.19	0.04	0.18
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	8	0.18	0.07	0.17
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	8	0.18	0.07	0.17
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	8	0.18	0.07	0.17
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	7	0.47	0.02	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	7	0.47	0.02	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	7	0.47	0.02	0.48

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	7	0.3	0.03	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	7	0.3	0.03	0.3
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	7	0.23	0.07	0.2
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	7	0.23	0.07	0.2
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	7	0.23	0.07	0.2
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	7	0.23	0.07	0.2
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	7	0.23	0.07	0.2
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	7	0.23	0.07	0.2
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	7	0.22	0.1	0.2
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	7	0.22	0.07	0.23
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	7	0.22	0.07	0.23
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	7	0.22	0.07	0.23
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	7	0.18	0.04	0.19
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	7	0.18	0.04	0.19
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	7	0.17	0.03	0.18
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	7	0.17	0.03	0.18
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	7	0.16	0.03	0.17
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	7	0.16	0.03	0.17
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	7	0.16	0.03	0.17
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	7	0.16	0.03	0.17
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	7	0.16	0.03	0.17
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	7	0.16	0.03	0.17
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	7	0.16	0.05	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	7	0.16	0.05	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	7	0.16	0.05	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	7	0.16	0.05	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	7	0.16	0.05	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	7	0.16	0.05	0.12
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	7	0.15	0.04	0.15
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	7	0.14	0.03	0.12
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD11	6	0.26	0.1	0.26
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD12	6	0.26	0.1	0.26
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD13	6	0.26	0.1	0.26
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD11	6	0.26	0.1	0.26
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD12	6	0.26	0.1	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD13	6	0.26	0.1	0.26
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD11	6	0.26	0.1	0.26
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD12	6	0.26	0.1	0.26
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD13	6	0.26	0.1	0.26
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG2	6	0.24	0.08	0.22
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG3	6	0.24	0.08	0.22
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG2	6	0.24	0.08	0.22
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG3	6	0.24	0.08	0.22
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG2	6	0.24	0.08	0.22
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG3	6	0.24	0.08	0.22
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG21	6	0.24	0.07	0.22
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG22	6	0.24	0.07	0.22
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG23	6	0.24	0.07	0.22
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE1	6	0.24	0.05	0.26
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE2	6	0.24	0.05	0.26
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE3	6	0.24	0.05	0.26
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE1	6	0.24	0.05	0.26
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE2	6	0.24	0.05	0.26
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE3	6	0.24	0.05	0.26
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD11	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD12	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD13	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD21	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD22	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD23	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD11	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD12	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD13	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD21	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD22	6	0.21	0.09	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD23	6	0.21	0.09	0.18
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG21	6	0.21	0.07	0.2
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG22	6	0.21	0.07	0.2
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG23	6	0.21	0.07	0.2
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD11	6	0.2	0.06	0.21
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD12	6	0.2	0.06	0.21
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD13	6	0.2	0.06	0.21
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD11	6	0.19	0.04	0.19
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD12	6	0.19	0.04	0.19
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD13	6	0.19	0.04	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD11	6	0.19	0.04	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD12	6	0.19	0.04	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD13	6	0.19	0.04	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD11	6	0.19	0.04	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD12	6	0.19	0.04	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD13	6	0.19	0.04	0.19
(1,492)	1:97:A:THR:HB	1:167:A:LEU:HG	6	0.17	0.04	0.17
(1,1224)	1:164:A:LYS:HB2	1:166:A:LYS:H	6	0.16	0.08	0.11
(1,1224)	1:164:A:LYS:HB3	1:166:A:LYS:H	6	0.16	0.08	0.11
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	6	0.16	0.03	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	6	0.16	0.03	0.15
(1,1506)	1:82:A:LEU:HD11	1:174:A:ASN:HA	6	0.16	0.06	0.14
(1,1506)	1:82:A:LEU:HD12	1:174:A:ASN:HA	6	0.16	0.06	0.14
(1,1506)	1:82:A:LEU:HD13	1:174:A:ASN:HA	6	0.16	0.06	0.14
(1,1506)	1:82:A:LEU:HD21	1:174:A:ASN:HA	6	0.16	0.06	0.14
(1,1506)	1:82:A:LEU:HD22	1:174:A:ASN:HA	6	0.16	0.06	0.14
(1,1506)	1:82:A:LEU:HD23	1:174:A:ASN:HA	6	0.16	0.06	0.14
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG11	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG12	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG13	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG21	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG22	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG23	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG11	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG12	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG13	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG21	6	0.15	0.03	0.15
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG22	6	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG23	6	0.15	0.03	0.15
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE2	6	0.13	0.04	0.12
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE3	6	0.13	0.04	0.12
(1,1331)	1:30:A:LEU:HD11	1:34:A:THR:H	6	0.13	0.02	0.13
(1,1331)	1:30:A:LEU:HD12	1:34:A:THR:H	6	0.13	0.02	0.13
(1,1331)	1:30:A:LEU:HD13	1:34:A:THR:H	6	0.13	0.02	0.13
(1,1331)	1:30:A:LEU:HD21	1:34:A:THR:H	6	0.13	0.02	0.13
(1,1331)	1:30:A:LEU:HD22	1:34:A:THR:H	6	0.13	0.02	0.13
(1,1331)	1:30:A:LEU:HD23	1:34:A:THR:H	6	0.13	0.02	0.13
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG12	6	0.13	0.02	0.12
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG13	6	0.13	0.02	0.12
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE1	5	0.36	0.08	0.38
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE2	5	0.36	0.08	0.38
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE3	5	0.36	0.08	0.38
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE1	5	0.36	0.08	0.38
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE2	5	0.36	0.08	0.38
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE3	5	0.36	0.08	0.38
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD2	5	0.3	0.03	0.33
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD3	5	0.3	0.03	0.33
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE2	5	0.24	0.12	0.21
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE3	5	0.24	0.12	0.21
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE2	5	0.24	0.12	0.21
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE3	5	0.24	0.12	0.21
(1,755)	1:175:A:TYR:HD1	1:179:A:GLU:HA	5	0.24	0.05	0.24
(1,755)	1:175:A:TYR:HD2	1:179:A:GLU:HA	5	0.24	0.05	0.24
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG21	5	0.23	0.08	0.24
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG22	5	0.23	0.08	0.24
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG23	5	0.23	0.08	0.24
(1,305)	1:149:A:PRO:HB3	1:152:A:THR:HB	5	0.2	0.07	0.17
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE2	5	0.19	0.1	0.14
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE3	5	0.19	0.1	0.14
(1,157)	1:45:A:ILE:HG21	1:125:A:VAL:HA	5	0.18	0.08	0.15
(1,157)	1:45:A:ILE:HG22	1:125:A:VAL:HA	5	0.18	0.08	0.15
(1,157)	1:45:A:ILE:HG23	1:125:A:VAL:HA	5	0.18	0.08	0.15
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE1	5	0.18	0.06	0.19
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE2	5	0.18	0.06	0.19
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE3	5	0.18	0.06	0.19
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE1	5	0.16	0.04	0.16
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE2	5	0.16	0.04	0.16
(1,542)	1:36:A:ILE:HD11	1:40:A:ARG:HB3	5	0.16	0.05	0.13
(1,542)	1:36:A:ILE:HD12	1:40:A:ARG:HB3	5	0.16	0.05	0.13
(1,542)	1:36:A:ILE:HD13	1:40:A:ARG:HB3	5	0.16	0.05	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,786)	1:66:A:PHE:HD1	1:132:A:LEU:HG	5	0.16	0.03	0.16
(1,786)	1:66:A:PHE:HD2	1:132:A:LEU:HG	5	0.16	0.03	0.16
(1,1018)	1:116:A:SER:HB2	1:118:A:MET:H	5	0.15	0.01	0.16
(1,1018)	1:116:A:SER:HB3	1:118:A:MET:H	5	0.15	0.01	0.16
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE1	5	0.13	0.03	0.12
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE2	5	0.13	0.03	0.12
(1,98)	1:33:A:GLU:HA	1:36:A:ILE:HB	5	0.13	0.01	0.12
(1,172)	1:99:A:ILE:HD11	1:118:A:MET:HA	4	0.28	0.1	0.31
(1,172)	1:99:A:ILE:HD12	1:118:A:MET:HA	4	0.28	0.1	0.31
(1,172)	1:99:A:ILE:HD13	1:118:A:MET:HA	4	0.28	0.1	0.31
(1,266)	1:180:A:LYS:HB2	1:186:A:PHE:HB2	4	0.26	0.06	0.24
(1,266)	1:180:A:LYS:HB3	1:186:A:PHE:HB2	4	0.26	0.06	0.24
(1,1220)	1:149:A:PRO:HB3	1:150:A:THR:H	4	0.23	0.06	0.2
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG12	4	0.22	0.03	0.23
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG13	4	0.22	0.03	0.23
(1,1477)	1:75:A:VAL:HG11	1:77:A:GLU:HA	4	0.2	0.14	0.14
(1,1477)	1:75:A:VAL:HG12	1:77:A:GLU:HA	4	0.2	0.14	0.14
(1,1477)	1:75:A:VAL:HG13	1:77:A:GLU:HA	4	0.2	0.14	0.14
(1,1477)	1:75:A:VAL:HG21	1:77:A:GLU:HA	4	0.2	0.14	0.14
(1,1477)	1:75:A:VAL:HG22	1:77:A:GLU:HA	4	0.2	0.14	0.14
(1,1477)	1:75:A:VAL:HG23	1:77:A:GLU:HA	4	0.2	0.14	0.14
(1,753)	1:175:A:TYR:HD1	1:180:A:LYS:H	4	0.2	0.04	0.22
(1,753)	1:175:A:TYR:HD2	1:180:A:LYS:H	4	0.2	0.04	0.22
(1,795)	1:66:A:PHE:HE1	1:132:A:LEU:HA	4	0.2	0.08	0.16
(1,795)	1:66:A:PHE:HE2	1:132:A:LEU:HA	4	0.2	0.08	0.16
(1,687)	1:55:A:ASP:HA	1:80:A:PHE:HZ	4	0.2	0.08	0.16
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD11	4	0.19	0.05	0.16
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD12	4	0.19	0.05	0.16
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD13	4	0.19	0.05	0.16
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB2	4	0.18	0.03	0.18
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB3	4	0.18	0.03	0.18
(1,774)	1:66:A:PHE:HD1	1:81:A:ILE:HA	4	0.18	0.01	0.18
(1,774)	1:66:A:PHE:HD2	1:81:A:ILE:HA	4	0.18	0.01	0.18
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE1	4	0.17	0.09	0.13
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE2	4	0.17	0.09	0.13
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE1	4	0.17	0.09	0.13
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE2	4	0.17	0.09	0.13
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG2	4	0.17	0.05	0.15
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG3	4	0.17	0.05	0.15
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE1	4	0.16	0.04	0.15
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE2	4	0.16	0.04	0.15
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE3	4	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE1	4	0.16	0.04	0.15
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE2	4	0.16	0.04	0.15
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE3	4	0.16	0.04	0.15
(1,189)	1:49:A:ILE:HA	1:132:A:LEU:HG	4	0.16	0.04	0.16
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD2	4	0.16	0.04	0.16
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD3	4	0.16	0.04	0.16
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD2	4	0.16	0.04	0.16
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD3	4	0.16	0.04	0.16
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD2	4	0.16	0.04	0.16
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD3	4	0.16	0.04	0.16
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD11	4	0.14	0.02	0.14
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD12	4	0.14	0.02	0.14
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD13	4	0.14	0.02	0.14
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD11	4	0.14	0.02	0.14
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD12	4	0.14	0.02	0.14
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD13	4	0.14	0.02	0.14
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE2	4	0.14	0.03	0.12
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE3	4	0.14	0.03	0.12
(1,739)	1:119:A:TYR:HE1	1:142:A:THR:HA	4	0.12	0.01	0.12
(1,739)	1:119:A:TYR:HE2	1:142:A:THR:HA	4	0.12	0.01	0.12
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG21	3	0.4	0.0	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG22	3	0.4	0.0	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG23	3	0.4	0.0	0.4
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG11	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG12	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG13	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG11	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG12	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG13	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG11	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG12	3	0.36	0.05	0.38
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG13	3	0.36	0.05	0.38
(1,1603)	1:99:A:ILE:HG12	1:118:A:MET:H	3	0.29	0.02	0.3
(1,1603)	1:99:A:ILE:HG13	1:118:A:MET:H	3	0.29	0.02	0.3
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE1	3	0.24	0.04	0.22
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE2	3	0.24	0.04	0.22
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE1	3	0.24	0.04	0.22
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE2	3	0.24	0.04	0.22
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE1	3	0.24	0.04	0.22
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE2	3	0.24	0.04	0.22
(1,1187)	1:116:A:SER:HA	1:152:A:THR:H	3	0.22	0.07	0.24
(1,866)	1:46:A:THR:HB	1:48:A:GLU:H	3	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD1	3	0.2	0.06	0.24
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD2	3	0.2	0.06	0.24
(1,400)	1:92:A:ALA:HB1	1:129:A:LEU:HG	3	0.19	0.08	0.16
(1,400)	1:92:A:ALA:HB2	1:129:A:LEU:HG	3	0.19	0.08	0.16
(1,400)	1:92:A:ALA:HB3	1:129:A:LEU:HG	3	0.19	0.08	0.16
(1,309)	1:118:A:MET:HE1	1:151:A:THR:HB	3	0.19	0.01	0.19
(1,309)	1:118:A:MET:HE2	1:151:A:THR:HB	3	0.19	0.01	0.19
(1,309)	1:118:A:MET:HE3	1:151:A:THR:HB	3	0.19	0.01	0.19
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG21	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG22	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG23	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG21	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG22	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG23	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG21	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG22	3	0.19	0.05	0.22
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG23	3	0.19	0.05	0.22
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD1	3	0.18	0.01	0.18
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD2	3	0.18	0.01	0.18
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE1	3	0.18	0.06	0.14
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE2	3	0.18	0.06	0.14
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE3	3	0.18	0.06	0.14
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD11	3	0.18	0.04	0.18
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD12	3	0.18	0.04	0.18
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD13	3	0.18	0.04	0.18
(1,121)	1:89:A:THR:HG21	1:171:A:HIS:HA	3	0.17	0.05	0.16
(1,121)	1:89:A:THR:HG22	1:171:A:HIS:HA	3	0.17	0.05	0.16
(1,121)	1:89:A:THR:HG23	1:171:A:HIS:HA	3	0.17	0.05	0.16
(1,419)	1:49:A:ILE:HG21	1:132:A:LEU:HB3	3	0.17	0.03	0.17
(1,419)	1:49:A:ILE:HG22	1:132:A:LEU:HB3	3	0.17	0.03	0.17
(1,419)	1:49:A:ILE:HG23	1:132:A:LEU:HB3	3	0.17	0.03	0.17
(1,692)	1:63:A:PHE:HB2	1:80:A:PHE:HZ	3	0.17	0.05	0.21
(1,692)	1:63:A:PHE:HB3	1:80:A:PHE:HZ	3	0.17	0.05	0.21
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG21	3	0.17	0.04	0.19
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG22	3	0.17	0.04	0.19
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG23	3	0.17	0.04	0.19
(1,21)	1:103:A:ALA:HA	1:109:A:THR:HB	3	0.17	0.02	0.16
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE1	3	0.17	0.05	0.14
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE2	3	0.17	0.05	0.14
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE3	3	0.17	0.05	0.14
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE1	3	0.17	0.05	0.14
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE2	3	0.17	0.05	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE3	3	0.17	0.05	0.14
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE1	3	0.17	0.05	0.14
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE2	3	0.17	0.05	0.14
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE3	3	0.17	0.05	0.14
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG21	3	0.16	0.06	0.14
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG22	3	0.16	0.06	0.14
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG23	3	0.16	0.06	0.14
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB2	3	0.16	0.06	0.13
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB3	3	0.16	0.06	0.13
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG11	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG12	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG13	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG21	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG22	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG23	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG11	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG12	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG13	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG21	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG22	3	0.16	0.01	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG23	3	0.16	0.01	0.16
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD21	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD22	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD23	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD21	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD22	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD23	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD21	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD22	3	0.16	0.02	0.16
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD23	3	0.16	0.02	0.16
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE1	3	0.15	0.03	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE2	3	0.15	0.03	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE3	3	0.15	0.03	0.13
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD11	3	0.15	0.04	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD12	3	0.15	0.04	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD13	3	0.15	0.04	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD21	3	0.15	0.04	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD22	3	0.15	0.04	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD23	3	0.15	0.04	0.15
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB2	3	0.14	0.03	0.13
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB3	3	0.14	0.03	0.13
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG2	3	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG3	3	0.14	0.03	0.13
(1,447)	1:97:A:THR:HG21	1:101:A:GLY:HA2	3	0.13	0.03	0.11
(1,447)	1:97:A:THR:HG22	1:101:A:GLY:HA2	3	0.13	0.03	0.11
(1,447)	1:97:A:THR:HG23	1:101:A:GLY:HA2	3	0.13	0.03	0.11
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB1	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB2	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB3	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB1	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB2	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB3	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB1	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB2	3	0.13	0.01	0.13
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB3	3	0.13	0.01	0.13
(1,200)	1:137:A:MET:HE1	1:141:A:VAL:HA	3	0.13	0.02	0.12
(1,200)	1:137:A:MET:HE2	1:141:A:VAL:HA	3	0.13	0.02	0.12
(1,200)	1:137:A:MET:HE3	1:141:A:VAL:HA	3	0.13	0.02	0.12
(1,1440)	1:61:A:VAL:HG11	1:80:A:PHE:HZ	3	0.13	0.0	0.13
(1,1440)	1:61:A:VAL:HG12	1:80:A:PHE:HZ	3	0.13	0.0	0.13
(1,1440)	1:61:A:VAL:HG13	1:80:A:PHE:HZ	3	0.13	0.0	0.13
(1,1440)	1:61:A:VAL:HG21	1:80:A:PHE:HZ	3	0.13	0.0	0.13
(1,1440)	1:61:A:VAL:HG22	1:80:A:PHE:HZ	3	0.13	0.0	0.13
(1,1440)	1:61:A:VAL:HG23	1:80:A:PHE:HZ	3	0.13	0.0	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD11	3	0.12	0.01	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD12	3	0.12	0.01	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD13	3	0.12	0.01	0.13
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD11	3	0.12	0.01	0.12
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD12	3	0.12	0.01	0.12
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD13	3	0.12	0.01	0.12
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	2	0.46	0.02	0.46
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	2	0.46	0.02	0.46
(1,1636)	1:107:A:LYS:HB2	1:108:A:LYS:HD2	2	0.4	0.05	0.4
(1,1636)	1:107:A:LYS:HB2	1:108:A:LYS:HD3	2	0.4	0.05	0.4
(1,1636)	1:107:A:LYS:HB3	1:108:A:LYS:HD2	2	0.4	0.05	0.4
(1,1636)	1:107:A:LYS:HB3	1:108:A:LYS:HD3	2	0.4	0.05	0.4
(1,1643)	1:109:A:THR:HA	1:115:A:PHE:HB2	2	0.38	0.04	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1643)	1:109:A:THR:HA	1:115:A:PHE:HB3	2	0.38	0.04	0.38
(1,1393)	1:45:A:ILE:HG12	1:92:A:ALA:HA	2	0.33	0.05	0.33
(1,1393)	1:45:A:ILE:HG13	1:92:A:ALA:HA	2	0.33	0.05	0.33
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG21	2	0.23	0.03	0.23
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG22	2	0.23	0.03	0.23
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG23	2	0.23	0.03	0.23
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD21	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD22	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD23	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD21	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD22	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD23	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD21	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD22	2	0.23	0.02	0.23
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD23	2	0.23	0.02	0.23
(1,1474)	1:70:A:GLU:HG2	1:71:A:THR:HA	2	0.22	0.11	0.22
(1,1474)	1:70:A:GLU:HG3	1:71:A:THR:HA	2	0.22	0.11	0.22
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG11	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG12	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG13	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG21	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG22	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG23	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG11	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG12	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG13	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG21	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG22	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG23	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG11	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG12	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG13	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG21	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG22	2	0.22	0.1	0.22
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG23	2	0.22	0.1	0.22
(1,1719)	1:141:A:VAL:HG11	1:162:A:ILE:HB	2	0.21	0.04	0.21
(1,1719)	1:141:A:VAL:HG12	1:162:A:ILE:HB	2	0.21	0.04	0.21
(1,1719)	1:141:A:VAL:HG13	1:162:A:ILE:HB	2	0.21	0.04	0.21
(1,1719)	1:141:A:VAL:HG21	1:162:A:ILE:HB	2	0.21	0.04	0.21
(1,1719)	1:141:A:VAL:HG22	1:162:A:ILE:HB	2	0.21	0.04	0.21
(1,1719)	1:141:A:VAL:HG23	1:162:A:ILE:HB	2	0.21	0.04	0.21
(1,552)	1:49:A:ILE:HG21	1:132:A:LEU:HG	2	0.21	0.08	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,552)	1:49:A:ILE:HG22	1:132:A:LEU:HG	2	0.21	0.08	0.21
(1,552)	1:49:A:ILE:HG23	1:132:A:LEU:HG	2	0.21	0.08	0.21
(1,1587)	1:96:A:VAL:HG11	1:164:A:LYS:H	2	0.2	0.02	0.2
(1,1587)	1:96:A:VAL:HG12	1:164:A:LYS:H	2	0.2	0.02	0.2
(1,1587)	1:96:A:VAL:HG13	1:164:A:LYS:H	2	0.2	0.02	0.2
(1,1587)	1:96:A:VAL:HG21	1:164:A:LYS:H	2	0.2	0.02	0.2
(1,1587)	1:96:A:VAL:HG22	1:164:A:LYS:H	2	0.2	0.02	0.2
(1,1587)	1:96:A:VAL:HG23	1:164:A:LYS:H	2	0.2	0.02	0.2
(1,738)	1:119:A:TYR:HE1	1:145:A:ALA:HA	2	0.2	0.01	0.2
(1,738)	1:119:A:TYR:HE2	1:145:A:ALA:HA	2	0.2	0.01	0.2
(1,802)	1:66:A:PHE:HE1	1:81:A:ILE:HB	2	0.2	0.02	0.2
(1,802)	1:66:A:PHE:HE2	1:81:A:ILE:HB	2	0.2	0.02	0.2
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD21	2	0.18	0.05	0.18
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD22	2	0.18	0.05	0.18
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD23	2	0.18	0.05	0.18
(1,747)	1:175:A:TYR:HE1	1:178:A:LEU:HG	2	0.18	0.08	0.18
(1,747)	1:175:A:TYR:HE2	1:178:A:LEU:HG	2	0.18	0.08	0.18
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE1	2	0.18	0.05	0.18
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE2	2	0.18	0.05	0.18
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE3	2	0.18	0.05	0.18
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD11	2	0.18	0.06	0.18
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD12	2	0.18	0.06	0.18
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD13	2	0.18	0.06	0.18
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG11	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG12	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG13	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG11	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG12	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG13	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG11	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG12	2	0.17	0.03	0.17
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG13	2	0.17	0.03	0.17
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD11	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD12	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD13	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD11	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD12	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD13	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD11	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD12	2	0.16	0.04	0.16
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD13	2	0.16	0.04	0.16
(1,700)	1:103:A:ALA:HB1	1:115:A:PHE:HD1	2	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,700)	1:103:A:ALA:HB1	1:115:A:PHE:HD2	2	0.16	0.03	0.16
(1,700)	1:103:A:ALA:HB2	1:115:A:PHE:HD1	2	0.16	0.03	0.16
(1,700)	1:103:A:ALA:HB2	1:115:A:PHE:HD2	2	0.16	0.03	0.16
(1,700)	1:103:A:ALA:HB3	1:115:A:PHE:HD1	2	0.16	0.03	0.16
(1,700)	1:103:A:ALA:HB3	1:115:A:PHE:HD2	2	0.16	0.03	0.16
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB1	2	0.16	0.02	0.16
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB2	2	0.16	0.02	0.16
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB3	2	0.16	0.02	0.16
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB1	2	0.16	0.02	0.16
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB2	2	0.16	0.02	0.16
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB3	2	0.16	0.02	0.16
(1,1788)	1:172:A:THR:HG21	1:191:A:CYS:HB2	2	0.16	0.03	0.16
(1,1788)	1:172:A:THR:HG21	1:191:A:CYS:HB3	2	0.16	0.03	0.16
(1,1788)	1:172:A:THR:HG22	1:191:A:CYS:HB2	2	0.16	0.03	0.16
(1,1788)	1:172:A:THR:HG22	1:191:A:CYS:HB3	2	0.16	0.03	0.16
(1,1788)	1:172:A:THR:HG23	1:191:A:CYS:HB2	2	0.16	0.03	0.16
(1,1788)	1:172:A:THR:HG23	1:191:A:CYS:HB3	2	0.16	0.03	0.16
(1,1584)	1:96:A:VAL:HG11	1:160:A:ALA:HA	2	0.16	0.02	0.16
(1,1584)	1:96:A:VAL:HG12	1:160:A:ALA:HA	2	0.16	0.02	0.16
(1,1584)	1:96:A:VAL:HG13	1:160:A:ALA:HA	2	0.16	0.02	0.16
(1,1584)	1:96:A:VAL:HG21	1:160:A:ALA:HA	2	0.16	0.02	0.16
(1,1584)	1:96:A:VAL:HG22	1:160:A:ALA:HA	2	0.16	0.02	0.16
(1,1584)	1:96:A:VAL:HG23	1:160:A:ALA:HA	2	0.16	0.02	0.16
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG21	2	0.15	0.04	0.15
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG22	2	0.15	0.04	0.15
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG23	2	0.15	0.04	0.15
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB1	2	0.15	0.03	0.15
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB2	2	0.15	0.03	0.15
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB3	2	0.15	0.03	0.15
(1,778)	1:66:A:PHE:HD1	1:132:A:LEU:HB2	2	0.14	0.03	0.14
(1,778)	1:66:A:PHE:HD2	1:132:A:LEU:HB2	2	0.14	0.03	0.14
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB1	2	0.14	0.02	0.14
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB2	2	0.14	0.02	0.14
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB3	2	0.14	0.02	0.14
(1,1060)	1:177:A:ALA:HB1	1:181:A:LYS:H	2	0.14	0.04	0.14
(1,1060)	1:177:A:ALA:HB2	1:181:A:LYS:H	2	0.14	0.04	0.14
(1,1060)	1:177:A:ALA:HB3	1:181:A:LYS:H	2	0.14	0.04	0.14
(1,1137)	1:172:A:THR:HG21	1:174:A:ASN:H	2	0.14	0.02	0.14
(1,1137)	1:172:A:THR:HG22	1:174:A:ASN:H	2	0.14	0.02	0.14
(1,1137)	1:172:A:THR:HG23	1:174:A:ASN:H	2	0.14	0.02	0.14
(1,1670)	1:123:A:LEU:HD11	1:141:A:VAL:HB	2	0.14	0.02	0.14
(1,1670)	1:123:A:LEU:HD12	1:141:A:VAL:HB	2	0.14	0.02	0.14

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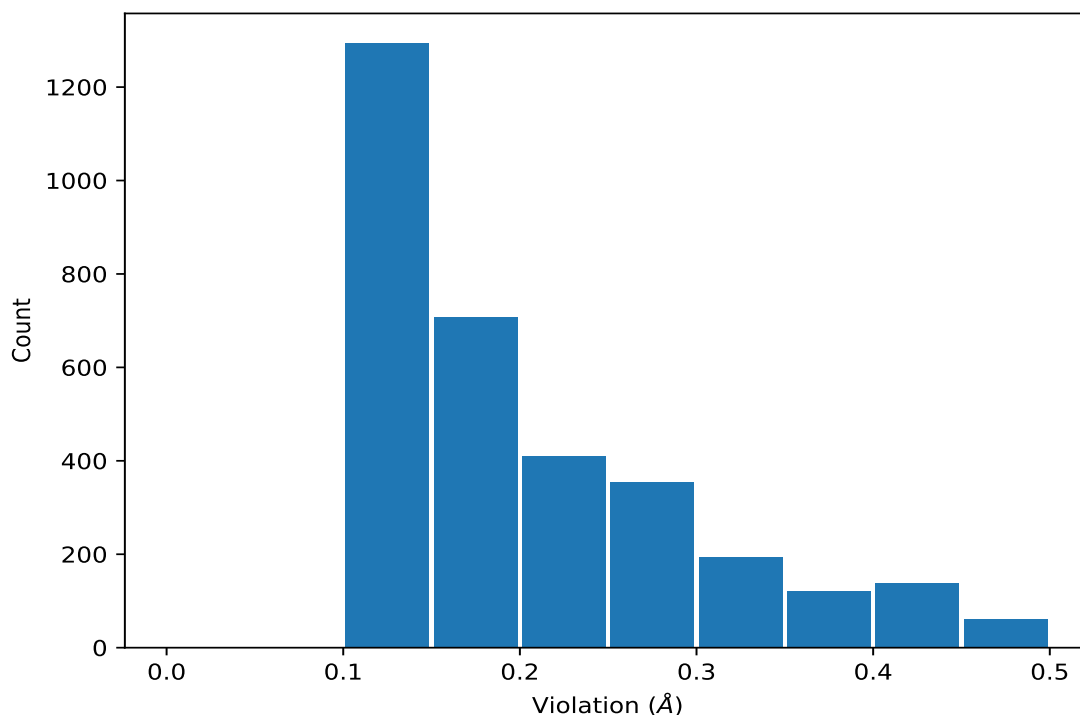
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1670)	1:123:A:LEU:HD13	1:141:A:VAL:HB	2	0.14	0.02	0.14
(1,1670)	1:123:A:LEU:HD21	1:141:A:VAL:HB	2	0.14	0.02	0.14
(1,1670)	1:123:A:LEU:HD22	1:141:A:VAL:HB	2	0.14	0.02	0.14
(1,1670)	1:123:A:LEU:HD23	1:141:A:VAL:HB	2	0.14	0.02	0.14
(1,229)	1:83:A:GLU:HG3	1:87:A:ARG:HD3	2	0.13	0.01	0.13
(1,1162)	1:109:A:THR:HB	1:116:A:SER:H	2	0.13	0.02	0.13
(1,1316)	1:29:A:GLY:HA2	1:31:A:LYS:HD2	2	0.13	0.0	0.13
(1,1316)	1:29:A:GLY:HA2	1:31:A:LYS:HD3	2	0.13	0.0	0.13
(1,1316)	1:29:A:GLY:HA3	1:31:A:LYS:HD2	2	0.13	0.0	0.13
(1,1316)	1:29:A:GLY:HA3	1:31:A:LYS:HD3	2	0.13	0.0	0.13
(1,462)	1:37:A:ILE:HG12	1:40:A:ARG:HB3	2	0.12	0.02	0.12
(1,462)	1:37:A:ILE:HG13	1:40:A:ARG:HB3	2	0.12	0.02	0.12
(1,1357)	1:36:A:ILE:HB	1:40:A:ARG:HD2	2	0.12	0.01	0.12
(1,1357)	1:36:A:ILE:HB	1:40:A:ARG:HD3	2	0.12	0.01	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD11	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD12	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD13	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD21	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD22	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD23	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD11	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD12	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD13	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD21	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD22	2	0.12	0.0	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD23	2	0.12	0.0	0.12
(1,90)	1:84:A:ALA:HA	1:87:A:ARG:HD2	2	0.11	0.0	0.11
(1,1300)	1:150:A:THR:HG21	1:152:A:THR:H	2	0.11	0.0	0.11
(1,1300)	1:150:A:THR:HG22	1:152:A:THR:H	2	0.11	0.0	0.11
(1,1300)	1:150:A:THR:HG23	1:152:A:THR:H	2	0.11	0.0	0.11
(1,1456)	1:65:A:ALA:H	1:76:A:SER:HB2	2	0.11	0.0	0.11
(1,1456)	1:65:A:ALA:H	1:76:A:SER:HB3	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 [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	10	0.49
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	10	0.49
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	10	0.49
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	10	0.49
(1,540)	1:161:A:LYS:HB3	1:162:A:ILE:HG12	1	0.49
(1,540)	1:161:A:LYS:HB3	1:162:A:ILE:HG13	1	0.49
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	5	0.49
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	5	0.49
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	5	0.49
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	7	0.49
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	7	0.49
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	7	0.49
(1,5)	1:151:A:THR:HA	1:152:A:THR:HA	9	0.49
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	4	0.48
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	4	0.48
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	4	0.48
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	4	0.48
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	4	0.48
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	4	0.48
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	4	0.48
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	4	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	3	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	3	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	3	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	4	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	4	0.48
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	4	0.48
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	4	0.47
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	4	0.47
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	4	0.47
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	4	0.47
(1,705)	1:80:A:PHE:HZ	1:81:A:ILE:HD11	10	0.47
(1,705)	1:80:A:PHE:HZ	1:81:A:ILE:HD12	10	0.47
(1,705)	1:80:A:PHE:HZ	1:81:A:ILE:HD13	10	0.47
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	2	0.47
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	2	0.47
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	2	0.47
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	2	0.47
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	2	0.47
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	2	0.47
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	2	0.47
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	2	0.47
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	2	0.47
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	6	0.46
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	6	0.46
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	6	0.46
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	9	0.46
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	9	0.46
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	9	0.46
(1,1636)	1:107:A:LYS:HB2	1:108:A:LYS:HD2	5	0.45
(1,1636)	1:107:A:LYS:HB2	1:108:A:LYS:HD3	5	0.45
(1,1636)	1:107:A:LYS:HB3	1:108:A:LYS:HD2	5	0.45
(1,1636)	1:107:A:LYS:HB3	1:108:A:LYS:HD3	5	0.45
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	10	0.45
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	10	0.45
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	10	0.45
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	10	0.45
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	10	0.45
(1,1477)	1:75:A:VAL:HG11	1:77:A:GLU:HA	3	0.44
(1,1477)	1:75:A:VAL:HG12	1:77:A:GLU:HA	3	0.44
(1,1477)	1:75:A:VAL:HG13	1:77:A:GLU:HA	3	0.44
(1,1477)	1:75:A:VAL:HG21	1:77:A:GLU:HA	3	0.44
(1,1477)	1:75:A:VAL:HG22	1:77:A:GLU:HA	3	0.44
(1,1477)	1:75:A:VAL:HG23	1:77:A:GLU:HA	3	0.44
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	4	0.44
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	4	0.44
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	4	0.44
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	4	0.44
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	4	0.44
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	4	0.44
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	4	0.44
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	4	0.44
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	4	0.44
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	8	0.44
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	8	0.44
(1,578)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	8	0.44
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	8	0.44
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	8	0.44
(1,578)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	8	0.44
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	8	0.44
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	8	0.44
(1,578)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	8	0.44
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	2	0.44
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	2	0.44
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	2	0.44
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG21	8	0.44
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG22	8	0.44
(1,460)	1:171:A:HIS:HB2	1:172:A:THR:HG23	8	0.44
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	7	0.44
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE1	9	0.44
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE2	9	0.44
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE3	9	0.44
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE1	9	0.44
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE2	9	0.44
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE3	9	0.44
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	4	0.44
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	4	0.44
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	3	0.43
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	3	0.43
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	3	0.43
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	3	0.43
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	8	0.42
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	8	0.42
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	8	0.42
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	8	0.42
(1,1643)	1:109:A:THR:HA	1:115:A:PHE:HB2	7	0.42
(1,1643)	1:109:A:THR:HA	1:115:A:PHE:HB3	7	0.42
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	10	0.42
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	10	0.42
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	10	0.42
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	10	0.42
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	10	0.42
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	10	0.42
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	10	0.42
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	10	0.42
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	10	0.42
(1,421)	1:45:A:ILE:HD11	1:92:A:ALA:HB1	6	0.42
(1,421)	1:45:A:ILE:HD11	1:92:A:ALA:HB2	6	0.42
(1,421)	1:45:A:ILE:HD11	1:92:A:ALA:HB3	6	0.42
(1,421)	1:45:A:ILE:HD12	1:92:A:ALA:HB1	6	0.42
(1,421)	1:45:A:ILE:HD12	1:92:A:ALA:HB2	6	0.42
(1,421)	1:45:A:ILE:HD12	1:92:A:ALA:HB3	6	0.42
(1,421)	1:45:A:ILE:HD13	1:92:A:ALA:HB1	6	0.42
(1,421)	1:45:A:ILE:HD13	1:92:A:ALA:HB2	6	0.42
(1,421)	1:45:A:ILE:HD13	1:92:A:ALA:HB3	6	0.42
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE1	1	0.42
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE2	1	0.42
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE3	1	0.42
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE1	1	0.42
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE2	1	0.42
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE3	1	0.42
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	1	0.41
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	1	0.41
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	1	0.41
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	1	0.41
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	1	0.41
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	1	0.41
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	1	0.41
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	1	0.41
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	1	0.41
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	1	0.41
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	1	0.41
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	1	0.41
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	1	0.41
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	1	0.41
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	1	0.41
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	1	0.41
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	1	0.41
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG11	8	0.41
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG12	8	0.41
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG13	8	0.41
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG11	8	0.41
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG12	8	0.41
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG13	8	0.41
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG11	8	0.41
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG12	8	0.41
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG13	8	0.41
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD11	2	0.41
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD12	2	0.41
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD13	2	0.41
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD11	2	0.41
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD12	2	0.41
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD13	2	0.41
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD11	2	0.41
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD12	2	0.41
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD13	2	0.41
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	5	0.4
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	5	0.4
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	5	0.4
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	5	0.4
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	5	0.4
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	5	0.4
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	5	0.4
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	5	0.4
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	5	0.4
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	5	0.4
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	5	0.4
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	5	0.4
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	5	0.4
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	5	0.4
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	5	0.4
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	5	0.4
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	5	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG21	1	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG22	1	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG23	1	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG21	3	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG22	3	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG23	3	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG21	8	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG22	8	0.4
(1,54)	1:71:A:THR:HA	1:71:A:THR:HG23	8	0.4
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	1	0.39
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	1	0.39
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	1	0.39
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	1	0.39
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	7	0.39
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	7	0.39
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	7	0.39
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	7	0.39
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE2	9	0.39
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE3	9	0.39
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE2	9	0.39
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE3	9	0.39
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG2	2	0.39
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG3	2	0.39
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG2	2	0.39
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG3	2	0.39
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG2	2	0.39
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG3	2	0.39
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD11	3	0.39
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD12	3	0.39
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD13	3	0.39
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD21	3	0.39
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD22	3	0.39
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD23	3	0.39
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD11	3	0.39
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD12	3	0.39
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD13	3	0.39
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD21	3	0.39
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD22	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD23	3	0.39
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	8	0.39
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	8	0.39
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	8	0.39
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	8	0.39
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	8	0.39
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	8	0.39
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	8	0.39
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	8	0.39
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	8	0.39
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	8	0.39
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	8	0.39
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	8	0.39
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	8	0.39
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	8	0.39
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	8	0.39
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	8	0.39
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	8	0.39
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	8	0.39
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	3	0.39
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	3	0.39
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	3	0.39
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	7	0.39
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	7	0.39
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	7	0.39
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	9	0.39
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	9	0.39
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	9	0.39
(1,172)	1:99:A:ILE:HD11	1:118:A:MET:HA	3	0.39
(1,172)	1:99:A:ILE:HD12	1:118:A:MET:HA	3	0.39
(1,172)	1:99:A:ILE:HD13	1:118:A:MET:HA	3	0.39
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE2	9	0.39
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE3	9	0.39
(1,1752)	1:154:A:GLU:HG2	1:157:A:LEU:HB2	2	0.38
(1,1752)	1:154:A:GLU:HG2	1:157:A:LEU:HB3	2	0.38
(1,1752)	1:154:A:GLU:HG3	1:157:A:LEU:HB2	2	0.38
(1,1752)	1:154:A:GLU:HG3	1:157:A:LEU:HB3	2	0.38
(1,1393)	1:45:A:ILE:HG12	1:92:A:ALA:HA	5	0.38
(1,1393)	1:45:A:ILE:HG13	1:92:A:ALA:HA	5	0.38
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG11	4	0.38
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG12	4	0.38
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG13	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG11	4	0.38
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG12	4	0.38
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG13	4	0.38
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG11	4	0.38
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG12	4	0.38
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG13	4	0.38
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	9	0.38
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE1	7	0.38
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE2	7	0.38
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE3	7	0.38
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE1	7	0.38
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE2	7	0.38
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE3	7	0.38
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	8	0.38
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	8	0.38
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	8	0.38
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	5	0.37
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	5	0.37
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	5	0.37
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	5	0.37
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE2	10	0.37
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE3	10	0.37
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE2	10	0.37
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE3	10	0.37
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	9	0.37
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	9	0.37
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	9	0.37
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	10	0.37
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	10	0.37
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	10	0.37
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG21	10	0.36
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG22	10	0.36
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG23	10	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	6	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	6	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	6	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	8	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	8	0.36
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	8	0.36
(1,266)	1:180:A:LYS:HB2	1:186:A:PHE:HB2	10	0.36
(1,266)	1:180:A:LYS:HB3	1:186:A:PHE:HB2	10	0.36
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE1	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE2	2	0.36
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE3	2	0.36
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE1	2	0.36
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE2	2	0.36
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE3	2	0.36
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	2	0.36
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	2	0.36
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	2	0.36
(1,1643)	1:109:A:THR:HA	1:115:A:PHE:HB2	6	0.35
(1,1643)	1:109:A:THR:HA	1:115:A:PHE:HB3	6	0.35
(1,1390)	1:45:A:ILE:HG12	1:91:A:VAL:H	7	0.35
(1,1390)	1:45:A:ILE:HG13	1:91:A:VAL:H	7	0.35
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	5	0.35
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	5	0.35
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	5	0.35
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	5	0.35
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	5	0.35
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	5	0.35
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	8	0.35
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	8	0.35
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	8	0.35
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	8	0.35
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	8	0.35
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	8	0.35
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	8	0.35
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	8	0.35
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	8	0.35
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	1	0.35
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	1	0.35
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	1	0.35
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	1	0.35
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	1	0.35
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	1	0.35
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	1	0.35
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	1	0.35
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	1	0.35
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	3	0.35
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	3	0.35
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	2	0.34
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	2	0.34
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	2	0.34
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1636)	1:107:A:LYS:HB2	1:108:A:LYS:HD2	8	0.34
(1,1636)	1:107:A:LYS:HB2	1:108:A:LYS:HD3	8	0.34
(1,1636)	1:107:A:LYS:HB3	1:108:A:LYS:HD2	8	0.34
(1,1636)	1:107:A:LYS:HB3	1:108:A:LYS:HD3	8	0.34
(1,687)	1:55:A:ASP:HA	1:80:A:PHE:HZ	10	0.34
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	8	0.34
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	8	0.34
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	8	0.34
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	3	0.34
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	3	0.34
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	3	0.34
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	3	0.34
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	3	0.34
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	3	0.34
(1,1474)	1:70:A:GLU:HG2	1:71:A:THR:HA	7	0.33
(1,1474)	1:70:A:GLU:HG3	1:71:A:THR:HA	7	0.33
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD2	7	0.33
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD3	7	0.33
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD2	8	0.33
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD3	8	0.33
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD2	10	0.33
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD3	10	0.33
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	6	0.33
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	6	0.33
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	6	0.33
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	6	0.33
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	6	0.33
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	6	0.33
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	6	0.33
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	6	0.33
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	6	0.33
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	6	0.33
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	6	0.33
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	6	0.33
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	6	0.33
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	6	0.33
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	6	0.33
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	6	0.33
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	6	0.33
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	6	0.33
(1,795)	1:66:A:PHE:HE1	1:132:A:LEU:HA	6	0.33
(1,795)	1:66:A:PHE:HE2	1:132:A:LEU:HA	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD11	7	0.33
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD12	7	0.33
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD13	7	0.33
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD11	7	0.33
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD12	7	0.33
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD13	7	0.33
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD11	7	0.33
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD12	7	0.33
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD13	7	0.33
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	7	0.33
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	8	0.33
(1,172)	1:99:A:ILE:HD11	1:118:A:MET:HA	9	0.33
(1,172)	1:99:A:ILE:HD12	1:118:A:MET:HA	9	0.33
(1,172)	1:99:A:ILE:HD13	1:118:A:MET:HA	9	0.33
(1,157)	1:45:A:ILE:HG21	1:125:A:VAL:HA	10	0.33
(1,157)	1:45:A:ILE:HG22	1:125:A:VAL:HA	10	0.33
(1,157)	1:45:A:ILE:HG23	1:125:A:VAL:HA	10	0.33
(1,1776)	1:163:A:MET:HB2	1:167:A:LEU:HD11	10	0.32
(1,1776)	1:163:A:MET:HB2	1:167:A:LEU:HD12	10	0.32
(1,1776)	1:163:A:MET:HB2	1:167:A:LEU:HD13	10	0.32
(1,1776)	1:163:A:MET:HB2	1:167:A:LEU:HD21	10	0.32
(1,1776)	1:163:A:MET:HB2	1:167:A:LEU:HD22	10	0.32
(1,1776)	1:163:A:MET:HB2	1:167:A:LEU:HD23	10	0.32
(1,1776)	1:163:A:MET:HB3	1:167:A:LEU:HD11	10	0.32
(1,1776)	1:163:A:MET:HB3	1:167:A:LEU:HD12	10	0.32
(1,1776)	1:163:A:MET:HB3	1:167:A:LEU:HD13	10	0.32
(1,1776)	1:163:A:MET:HB3	1:167:A:LEU:HD21	10	0.32
(1,1776)	1:163:A:MET:HB3	1:167:A:LEU:HD22	10	0.32
(1,1776)	1:163:A:MET:HB3	1:167:A:LEU:HD23	10	0.32
(1,1539)	1:86:A:VAL:HG11	1:174:A:ASN:HA	2	0.32
(1,1539)	1:86:A:VAL:HG12	1:174:A:ASN:HA	2	0.32
(1,1539)	1:86:A:VAL:HG13	1:174:A:ASN:HA	2	0.32
(1,1539)	1:86:A:VAL:HG21	1:174:A:ASN:HA	2	0.32
(1,1539)	1:86:A:VAL:HG22	1:174:A:ASN:HA	2	0.32
(1,1539)	1:86:A:VAL:HG23	1:174:A:ASN:HA	2	0.32
(1,1220)	1:149:A:PRO:HB3	1:150:A:THR:H	3	0.32
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE1	1	0.32
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE2	1	0.32
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE1	1	0.32
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE2	1	0.32
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	5	0.32
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	5	0.32
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	5	0.32
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	5	0.32
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	5	0.32
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	5	0.32
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	5	0.32
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	5	0.32
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG21	4	0.32
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG22	4	0.32
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG23	4	0.32
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	10	0.32
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	10	0.32
(1,305)	1:149:A:PRO:HB3	1:152:A:THR:HB	1	0.32
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG21	5	0.32
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG22	5	0.32
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG23	5	0.32
(1,1603)	1:99:A:ILE:HG12	1:118:A:MET:H	3	0.31
(1,1603)	1:99:A:ILE:HG13	1:118:A:MET:H	3	0.31
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG11	8	0.31
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG12	8	0.31
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG13	8	0.31
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG21	8	0.31
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG22	8	0.31
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG23	8	0.31
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG11	8	0.31
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG12	8	0.31
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG13	8	0.31
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG21	8	0.31
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG22	8	0.31
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG23	8	0.31
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG11	8	0.31
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG12	8	0.31
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG13	8	0.31
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG21	8	0.31
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG22	8	0.31
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG23	8	0.31
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	10	0.31
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	10	0.31
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	10	0.31
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	10	0.31
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	10	0.31
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	10	0.31
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	10	0.31
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	10	0.31
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	10	0.31
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	10	0.31
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	10	0.31
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	10	0.31
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	10	0.31
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	10	0.31
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	10	0.31
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	10	0.31
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	10	0.31
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	1	0.31
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	1	0.31
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	1	0.31
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	1	0.31
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	1	0.31
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	1	0.31
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	1	0.31
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	1	0.31
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	1	0.31
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	4	0.31
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	4	0.31
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	5	0.31
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	5	0.31
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	9	0.31
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	9	0.31
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	4	0.31
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	7	0.31
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	7	0.31
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	7	0.31
(1,15)	1:116:A:SER:HA	1:150:A:THR:HG21	9	0.31
(1,15)	1:116:A:SER:HA	1:150:A:THR:HG22	9	0.31
(1,15)	1:116:A:SER:HA	1:150:A:THR:HG23	9	0.31
(1,1603)	1:99:A:ILE:HG12	1:118:A:MET:H	10	0.3
(1,1603)	1:99:A:ILE:HG13	1:118:A:MET:H	10	0.3
(1,1224)	1:164:A:LYS:HB2	1:166:A:LYS:H	8	0.3
(1,1224)	1:164:A:LYS:HB3	1:166:A:LYS:H	8	0.3
(1,1187)	1:116:A:SER:HA	1:152:A:THR:H	4	0.3
(1,755)	1:175:A:TYR:HD1	1:179:A:GLU:HA	5	0.3
(1,755)	1:175:A:TYR:HD2	1:179:A:GLU:HA	5	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	2	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	2	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	2	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	2	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	2	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	2	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	2	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	2	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	6	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	6	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	6	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	6	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	6	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	6	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	6	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	6	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	6	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	9	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	9	0.3
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	9	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	9	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	9	0.3
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	9	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	9	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	9	0.3
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	9	0.3
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG11	5	0.3
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG12	5	0.3
(1,558)	1:45:A:ILE:HD11	1:91:A:VAL:HG13	5	0.3
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG11	5	0.3
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG12	5	0.3
(1,558)	1:45:A:ILE:HD12	1:91:A:VAL:HG13	5	0.3
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG11	5	0.3
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG12	5	0.3
(1,558)	1:45:A:ILE:HD13	1:91:A:VAL:HG13	5	0.3
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	2	0.3
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	2	0.3
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	2	0.3
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	5	0.3
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	5	0.3
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	5	0.3
(1,400)	1:92:A:ALA:HB1	1:129:A:LEU:HG	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:92:A:ALA:HB2	1:129:A:LEU:HG	6	0.3
(1,400)	1:92:A:ALA:HB3	1:129:A:LEU:HG	6	0.3
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	6	0.3
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	6	0.3
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	6	0.3
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	6	0.3
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	6	0.3
(1,1395)	1:45:A:ILE:HD11	1:91:A:VAL:HG11	5	0.29
(1,1395)	1:45:A:ILE:HD11	1:91:A:VAL:HG12	5	0.29
(1,1395)	1:45:A:ILE:HD11	1:91:A:VAL:HG13	5	0.29
(1,1395)	1:45:A:ILE:HD11	1:91:A:VAL:HG21	5	0.29
(1,1395)	1:45:A:ILE:HD11	1:91:A:VAL:HG22	5	0.29
(1,1395)	1:45:A:ILE:HD11	1:91:A:VAL:HG23	5	0.29
(1,1395)	1:45:A:ILE:HD12	1:91:A:VAL:HG11	5	0.29
(1,1395)	1:45:A:ILE:HD12	1:91:A:VAL:HG12	5	0.29
(1,1395)	1:45:A:ILE:HD12	1:91:A:VAL:HG13	5	0.29
(1,1395)	1:45:A:ILE:HD12	1:91:A:VAL:HG21	5	0.29
(1,1395)	1:45:A:ILE:HD12	1:91:A:VAL:HG22	5	0.29
(1,1395)	1:45:A:ILE:HD12	1:91:A:VAL:HG23	5	0.29
(1,1395)	1:45:A:ILE:HD13	1:91:A:VAL:HG11	5	0.29
(1,1395)	1:45:A:ILE:HD13	1:91:A:VAL:HG12	5	0.29
(1,1395)	1:45:A:ILE:HD13	1:91:A:VAL:HG13	5	0.29
(1,1395)	1:45:A:ILE:HD13	1:91:A:VAL:HG21	5	0.29
(1,1395)	1:45:A:ILE:HD13	1:91:A:VAL:HG22	5	0.29
(1,1395)	1:45:A:ILE:HD13	1:91:A:VAL:HG23	5	0.29
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	9	0.29
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	9	0.29
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	9	0.29
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE1	1	0.29
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE2	1	0.29
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE1	1	0.29
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE2	1	0.29
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE1	1	0.29
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE2	1	0.29
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	3	0.29
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	3	0.29
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	2	0.29
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	2	0.29
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	2	0.29
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	2	0.29
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	2	0.29
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	7	0.29
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	7	0.29
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	7	0.29
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	7	0.29
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	7	0.29
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	7	0.29
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	7	0.29
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	7	0.29
(1,552)	1:49:A:ILE:HG21	1:132:A:LEU:HG	4	0.29
(1,552)	1:49:A:ILE:HG22	1:132:A:LEU:HG	4	0.29
(1,552)	1:49:A:ILE:HG23	1:132:A:LEU:HG	4	0.29
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	8	0.29
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	8	0.29
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	8	0.29
(1,293)	1:125:A:VAL:HG11	1:128:A:PRO:HB3	10	0.29
(1,293)	1:125:A:VAL:HG12	1:128:A:PRO:HB3	10	0.29
(1,293)	1:125:A:VAL:HG13	1:128:A:PRO:HB3	10	0.29
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	2	0.29
(1,172)	1:99:A:ILE:HD11	1:118:A:MET:HA	10	0.29
(1,172)	1:99:A:ILE:HD12	1:118:A:MET:HA	10	0.29
(1,172)	1:99:A:ILE:HD13	1:118:A:MET:HA	10	0.29
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG21	7	0.29
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG22	7	0.29
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG23	7	0.29
(1,39)	1:77:A:GLU:HA	1:77:A:GLU:HG2	2	0.29
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG2	4	0.28
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG3	4	0.28
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG2	4	0.28
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG3	4	0.28
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG2	4	0.28
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG3	4	0.28
(1,1506)	1:82:A:LEU:HD11	1:174:A:ASN:HA	3	0.28
(1,1506)	1:82:A:LEU:HD12	1:174:A:ASN:HA	3	0.28
(1,1506)	1:82:A:LEU:HD13	1:174:A:ASN:HA	3	0.28
(1,1506)	1:82:A:LEU:HD21	1:174:A:ASN:HA	3	0.28
(1,1506)	1:82:A:LEU:HD22	1:174:A:ASN:HA	3	0.28
(1,1506)	1:82:A:LEU:HD23	1:174:A:ASN:HA	3	0.28
(1,1393)	1:45:A:ILE:HG12	1:92:A:ALA:HA	4	0.28
(1,1393)	1:45:A:ILE:HG13	1:92:A:ALA:HA	4	0.28
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	9	0.28
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	9	0.28
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	9	0.28
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	9	0.28
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	9	0.28
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	9	0.28
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	9	0.28
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	9	0.28
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	9	0.28
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	9	0.28
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	9	0.28
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	2	0.28
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	2	0.28
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	2	0.28
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	3	0.28
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	3	0.28
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG21	9	0.28
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG22	9	0.28
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG23	9	0.28
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE1	3	0.28
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE2	3	0.28
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE3	3	0.28
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE1	3	0.28
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE2	3	0.28
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE3	3	0.28
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD11	1	0.28
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD12	1	0.28
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD13	1	0.28
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	2	0.28
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	2	0.28
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	2	0.28
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	2	0.28
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	2	0.28
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	2	0.28
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	2	0.28
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	2	0.28
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	2	0.28
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	1	0.28
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	1	0.28
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	2	0.28
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	2	0.28
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	5	0.28
(1,1603)	1:99:A:ILE:HG12	1:118:A:MET:H	9	0.27
(1,1603)	1:99:A:ILE:HG13	1:118:A:MET:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD11	7	0.27
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD12	7	0.27
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD13	7	0.27
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD21	7	0.27
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD22	7	0.27
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD23	7	0.27
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD11	7	0.27
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD12	7	0.27
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD13	7	0.27
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD21	7	0.27
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD22	7	0.27
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD23	7	0.27
(1,755)	1:175:A:TYR:HD1	1:179:A:GLU:HA	10	0.27
(1,755)	1:175:A:TYR:HD2	1:179:A:GLU:HA	10	0.27
(1,747)	1:175:A:TYR:HE1	1:178:A:LEU:HG	10	0.27
(1,747)	1:175:A:TYR:HE2	1:178:A:LEU:HG	10	0.27
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	5	0.27
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	5	0.27
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE1	9	0.27
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE2	9	0.27
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE3	9	0.27
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE1	9	0.27
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE2	9	0.27
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE3	9	0.27
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE1	10	0.27
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE2	10	0.27
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE3	10	0.27
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE1	10	0.27
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE2	10	0.27
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE3	10	0.27
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD11	3	0.27
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD12	3	0.27
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD13	3	0.27
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD11	3	0.27
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD12	3	0.27
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD13	3	0.27
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD11	3	0.27
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD12	3	0.27
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD13	3	0.27
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	7	0.27
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	7	0.27
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	2	0.27
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	2	0.27
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	2	0.27
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	1	0.27
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD11	2	0.27
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD12	2	0.27
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD13	2	0.27
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	9	0.26
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	9	0.26
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	9	0.26
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	9	0.26
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	9	0.26
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	9	0.26
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD2	2	0.26
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD3	2	0.26
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD2	4	0.26
(1,1377)	1:40:A:ARG:HA	1:40:A:ARG:HD3	4	0.26
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	1	0.26
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	1	0.26
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	1	0.26
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	4	0.26
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	4	0.26
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	2	0.26
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	2	0.26
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	2	0.26
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	2	0.26
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	2	0.26
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	2	0.26
(1,695)	1:61:A:VAL:HG21	1:80:A:PHE:HZ	10	0.26
(1,695)	1:61:A:VAL:HG22	1:80:A:PHE:HZ	10	0.26
(1,695)	1:61:A:VAL:HG23	1:80:A:PHE:HZ	10	0.26
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	10	0.26
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	10	0.26
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	10	0.26
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	3	0.26
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	6	0.26
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG21	10	0.26
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG22	10	0.26
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG23	10	0.26
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG21	7	0.26
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG22	7	0.26
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG23	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE1	4	0.26
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE2	4	0.26
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE3	4	0.26
(1,266)	1:180:A:LYS:HB2	1:186:A:PHE:HB2	8	0.26
(1,266)	1:180:A:LYS:HB3	1:186:A:PHE:HB2	8	0.26
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	6	0.26
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE1	4	0.26
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE2	4	0.26
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE3	4	0.26
(1,1719)	1:141:A:VAL:HG11	1:162:A:ILE:HB	5	0.25
(1,1719)	1:141:A:VAL:HG12	1:162:A:ILE:HB	5	0.25
(1,1719)	1:141:A:VAL:HG13	1:162:A:ILE:HB	5	0.25
(1,1719)	1:141:A:VAL:HG21	1:162:A:ILE:HB	5	0.25
(1,1719)	1:141:A:VAL:HG22	1:162:A:ILE:HB	5	0.25
(1,1719)	1:141:A:VAL:HG23	1:162:A:ILE:HB	5	0.25
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG2	2	0.25
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG3	2	0.25
(1,1570)	1:93:A:GLU:HB2	1:167:A:LEU:HB2	10	0.25
(1,1570)	1:93:A:GLU:HB2	1:167:A:LEU:HB3	10	0.25
(1,1570)	1:93:A:GLU:HB3	1:167:A:LEU:HB2	10	0.25
(1,1570)	1:93:A:GLU:HB3	1:167:A:LEU:HB3	10	0.25
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	9	0.25
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	9	0.25
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	9	0.25
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	9	0.25
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	9	0.25
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	9	0.25
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	9	0.25
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	9	0.25
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	9	0.25
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	9	0.25
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	9	0.25
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	9	0.25
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	9	0.25
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	9	0.25
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	9	0.25
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	9	0.25
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	9	0.25
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	9	0.25
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB2	9	0.25
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB3	9	0.25
(1,931)	1:152:A:THR:H	1:156:A:ILE:H	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	6	0.25
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	6	0.25
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	6	0.25
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	8	0.25
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	8	0.25
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG21	1	0.25
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG22	1	0.25
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG23	1	0.25
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE1	2	0.25
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE2	2	0.25
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE3	2	0.25
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE1	2	0.25
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE2	2	0.25
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE3	2	0.25
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD1	9	0.25
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD2	9	0.25
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD21	4	0.25
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD22	4	0.25
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD23	4	0.25
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD21	4	0.25
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD22	4	0.25
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD23	4	0.25
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD21	4	0.25
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD22	4	0.25
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD23	4	0.25
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	3	0.25
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	3	0.25
(1,577)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	3	0.25
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	3	0.25
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	3	0.25
(1,577)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	3	0.25
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	3	0.25
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	3	0.25
(1,577)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	3	0.25
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD11	6	0.25
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD12	6	0.25
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD13	6	0.25
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD11	6	0.25
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD12	6	0.25
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD13	6	0.25
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD11	6	0.25
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD12	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD13	6	0.25
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	5	0.25
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	5	0.25
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	5	0.25
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	7	0.25
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	7	0.25
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	10	0.25
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD11	7	0.25
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD12	7	0.25
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD13	7	0.25
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	10	0.24
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	10	0.24
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG12	3	0.24
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG13	3	0.24
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG12	6	0.24
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG13	6	0.24
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG2	7	0.24
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG3	7	0.24
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG2	7	0.24
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG3	7	0.24
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG2	7	0.24
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG3	7	0.24
(1,1224)	1:164:A:LYS:HB2	1:166:A:LYS:H	7	0.24
(1,1224)	1:164:A:LYS:HB3	1:166:A:LYS:H	7	0.24
(1,1187)	1:116:A:SER:HA	1:152:A:THR:H	3	0.24
(1,755)	1:175:A:TYR:HD1	1:179:A:GLU:HA	3	0.24
(1,755)	1:175:A:TYR:HD2	1:179:A:GLU:HA	3	0.24
(1,755)	1:175:A:TYR:HD1	1:179:A:GLU:HA	4	0.24
(1,755)	1:175:A:TYR:HD2	1:179:A:GLU:HA	4	0.24
(1,753)	1:175:A:TYR:HD1	1:180:A:LYS:H	1	0.24
(1,753)	1:175:A:TYR:HD2	1:180:A:LYS:H	1	0.24
(1,753)	1:175:A:TYR:HD1	1:180:A:LYS:H	4	0.24
(1,753)	1:175:A:TYR:HD2	1:180:A:LYS:H	4	0.24
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	2	0.24
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	2	0.24
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG21	4	0.24
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG22	4	0.24
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG23	4	0.24
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD1	2	0.24
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD2	2	0.24
(1,658)	1:121:A:MET:H	1:121:A:MET:HE1	4	0.24
(1,658)	1:121:A:MET:H	1:121:A:MET:HE2	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:121:A:MET:H	1:121:A:MET:HE3	4	0.24
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	3	0.24
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	3	0.24
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	3	0.24
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	3	0.24
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	3	0.24
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	3	0.24
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	3	0.24
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	3	0.24
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	3	0.24
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD11	7	0.24
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD12	7	0.24
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD13	7	0.24
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD11	7	0.24
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD12	7	0.24
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD13	7	0.24
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD11	7	0.24
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD12	7	0.24
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD13	7	0.24
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE1	10	0.24
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE2	10	0.24
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE3	10	0.24
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE1	10	0.24
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE2	10	0.24
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE3	10	0.24
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE1	10	0.24
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE2	10	0.24
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE3	10	0.24
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD21	9	0.24
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD22	9	0.24
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD23	9	0.24
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	5	0.24
(1,305)	1:149:A:PRO:HB3	1:152:A:THR:HB	9	0.24
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG21	6	0.24
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG22	6	0.24
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG23	6	0.24
(1,121)	1:89:A:THR:HG21	1:171:A:HIS:HA	9	0.24
(1,121)	1:89:A:THR:HG22	1:171:A:HIS:HA	9	0.24
(1,121)	1:89:A:THR:HG23	1:171:A:HIS:HA	9	0.24
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	5	0.23
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	5	0.23
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	9	0.23
(1,1651)	1:115:A:PHE:HB2	1:156:A:ILE:HG12	2	0.23
(1,1651)	1:115:A:PHE:HB2	1:156:A:ILE:HG13	2	0.23
(1,1651)	1:115:A:PHE:HB3	1:156:A:ILE:HG12	2	0.23
(1,1651)	1:115:A:PHE:HB3	1:156:A:ILE:HG13	2	0.23
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE1	6	0.23
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE2	6	0.23
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE3	6	0.23
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE1	6	0.23
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE2	6	0.23
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE3	6	0.23
(1,1220)	1:149:A:PRO:HB3	1:150:A:THR:H	6	0.23
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	3	0.23
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	3	0.23
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	5	0.23
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	5	0.23
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	8	0.23
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	8	0.23
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	8	0.23
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG21	5	0.23
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG22	5	0.23
(1,654)	1:139:A:LYS:H	1:140:A:THR:HG23	5	0.23
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	1	0.23
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	1	0.23
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	1	0.23
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG21	10	0.23
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG22	10	0.23
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG23	10	0.23
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG21	10	0.23
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG22	10	0.23
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG23	10	0.23
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG21	10	0.23
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG22	10	0.23
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG23	10	0.23
(1,542)	1:36:A:ILE:HD11	1:40:A:ARG:HB3	7	0.23
(1,542)	1:36:A:ILE:HD12	1:40:A:ARG:HB3	7	0.23
(1,542)	1:36:A:ILE:HD13	1:40:A:ARG:HB3	7	0.23
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	8	0.23
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	8	0.23
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	8	0.23
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	2	0.23
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	2	0.23
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	6	0.23
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	6	0.23
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	6	0.23
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG21	3	0.23
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG22	3	0.23
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG23	3	0.23
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE1	1	0.23
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE2	1	0.23
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE3	1	0.23
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE1	3	0.23
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE2	3	0.23
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE3	3	0.23
(1,134)	1:83:A:GLU:HA	1:86:A:VAL:HG21	2	0.23
(1,134)	1:83:A:GLU:HA	1:86:A:VAL:HG22	2	0.23
(1,134)	1:83:A:GLU:HA	1:86:A:VAL:HG23	2	0.23
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD11	3	0.23
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD12	3	0.23
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD13	3	0.23
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE2	10	0.23
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE3	10	0.23
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	6	0.22
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	6	0.22
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	6	0.22
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	6	0.22
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG12	7	0.22
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG13	7	0.22
(1,1587)	1:96:A:VAL:HG11	1:164:A:LYS:H	7	0.22
(1,1587)	1:96:A:VAL:HG12	1:164:A:LYS:H	7	0.22
(1,1587)	1:96:A:VAL:HG13	1:164:A:LYS:H	7	0.22
(1,1587)	1:96:A:VAL:HG21	1:164:A:LYS:H	7	0.22
(1,1587)	1:96:A:VAL:HG22	1:164:A:LYS:H	7	0.22
(1,1587)	1:96:A:VAL:HG23	1:164:A:LYS:H	7	0.22
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	7	0.22
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	7	0.22
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	7	0.22
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	7	0.22
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	7	0.22
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	7	0.22
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	7	0.22
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	7	0.22
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	7	0.22
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	7	0.22
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	7	0.22
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	7	0.22
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	7	0.22
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	7	0.22
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	7	0.22
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	7	0.22
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	7	0.22
(1,859)	1:115:A:PHE:HD1	1:153:A:ALA:H	9	0.22
(1,859)	1:115:A:PHE:HD2	1:153:A:ALA:H	9	0.22
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE1	10	0.22
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE2	10	0.22
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE1	10	0.22
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE2	10	0.22
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE1	10	0.22
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE2	10	0.22
(1,802)	1:66:A:PHE:HE1	1:81:A:ILE:HB	5	0.22
(1,802)	1:66:A:PHE:HE2	1:81:A:ILE:HB	5	0.22
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	6	0.22
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	6	0.22
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD11	1	0.22
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD12	1	0.22
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD13	1	0.22
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG21	8	0.22
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG22	8	0.22
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG23	8	0.22
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG21	8	0.22
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG22	8	0.22
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG23	8	0.22
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG21	8	0.22
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG22	8	0.22
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG23	8	0.22
(1,492)	1:97:A:THR:HB	1:167:A:LEU:HG	2	0.22
(1,492)	1:97:A:THR:HB	1:167:A:LEU:HG	9	0.22
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	1	0.22
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	1	0.22
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	1	0.22
(1,443)	1:30:A:LEU:HA	1:34:A:THR:HG21	9	0.22
(1,443)	1:30:A:LEU:HA	1:34:A:THR:HG22	9	0.22
(1,443)	1:30:A:LEU:HA	1:34:A:THR:HG23	9	0.22
(1,266)	1:180:A:LYS:HB2	1:186:A:PHE:HB2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:180:A:LYS:HB3	1:186:A:PHE:HB2	7	0.22
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE1	5	0.22
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE2	5	0.22
(1,243)	1:121:A:MET:HG2	1:122:A:MET:HE3	5	0.22
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE1	5	0.22
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE2	5	0.22
(1,243)	1:121:A:MET:HG3	1:122:A:MET:HE3	5	0.22
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD11	4	0.22
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD12	4	0.22
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD13	4	0.22
(1,91)	1:91:A:VAL:HA	1:94:A:LYS:HE2	2	0.22
(1,91)	1:91:A:VAL:HA	1:94:A:LYS:HE3	2	0.22
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	7	0.21
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	7	0.21
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE2	7	0.21
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE3	7	0.21
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE2	7	0.21
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE3	7	0.21
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	7	0.21
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	7	0.21
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	7	0.21
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	7	0.21
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	7	0.21
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	7	0.21
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	7	0.21
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	7	0.21
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	7	0.21
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	7	0.21
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	7	0.21
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	7	0.21
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	7	0.21
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	7	0.21
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	7	0.21
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	7	0.21
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	7	0.21
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	7	0.21
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	8	0.21
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	8	0.21
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	9	0.21
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	9	0.21
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	9	0.21
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	9	0.21
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	9	0.21
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB2	10	0.21
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB3	10	0.21
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	3	0.21
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	7	0.21
(1,866)	1:46:A:THR:HB	1:48:A:GLU:H	5	0.21
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE1	2	0.21
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE2	2	0.21
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE1	9	0.21
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE2	9	0.21
(1,753)	1:175:A:TYR:HD1	1:180:A:LYS:H	9	0.21
(1,753)	1:175:A:TYR:HD2	1:180:A:LYS:H	9	0.21
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	9	0.21
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	9	0.21
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	1	0.21
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	1	0.21
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	7	0.21
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	7	0.21
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE1	8	0.21
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE2	8	0.21
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE3	8	0.21
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE1	8	0.21
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE2	8	0.21
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE3	8	0.21
(1,692)	1:63:A:PHE:HB2	1:80:A:PHE:HZ	2	0.21
(1,692)	1:63:A:PHE:HB3	1:80:A:PHE:HZ	2	0.21
(1,692)	1:63:A:PHE:HB2	1:80:A:PHE:HZ	9	0.21
(1,692)	1:63:A:PHE:HB3	1:80:A:PHE:HZ	9	0.21
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	2	0.21
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	2	0.21
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD21	6	0.21
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD22	6	0.21
(1,596)	1:56:A:ALA:HB1	1:132:A:LEU:HD23	6	0.21
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD21	6	0.21
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD22	6	0.21
(1,596)	1:56:A:ALA:HB2	1:132:A:LEU:HD23	6	0.21
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD21	6	0.21
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD22	6	0.21
(1,596)	1:56:A:ALA:HB3	1:132:A:LEU:HD23	6	0.21
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD11	1	0.21
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD12	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD13	1	0.21
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD11	1	0.21
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD12	1	0.21
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD13	1	0.21
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD11	1	0.21
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD12	1	0.21
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD13	1	0.21
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG21	9	0.21
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG22	9	0.21
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG23	9	0.21
(1,419)	1:49:A:ILE:HG21	1:132:A:LEU:HB3	3	0.21
(1,419)	1:49:A:ILE:HG22	1:132:A:LEU:HB3	3	0.21
(1,419)	1:49:A:ILE:HG23	1:132:A:LEU:HB3	3	0.21
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	6	0.21
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	3	0.21
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	4	0.2
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	4	0.2
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	8	0.2
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	8	0.2
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD2	6	0.2
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD3	6	0.2
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD2	6	0.2
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD3	6	0.2
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD2	6	0.2
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD3	6	0.2
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG2	5	0.2
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG3	5	0.2
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG2	5	0.2
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG3	5	0.2
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG2	5	0.2
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG3	5	0.2
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	3	0.2
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	3	0.2
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	7	0.2
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	7	0.2
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	3	0.2
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	3	0.2
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	3	0.2
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	3	0.2
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	3	0.2
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	3	0.2
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	3	0.2
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	3	0.2
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	3	0.2
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	3	0.2
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	3	0.2
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	2	0.2
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	2	0.2
(1,1072)	1:45:A:ILE:HD11	1:96:A:VAL:H	6	0.2
(1,1072)	1:45:A:ILE:HD12	1:96:A:VAL:H	6	0.2
(1,1072)	1:45:A:ILE:HD13	1:96:A:VAL:H	6	0.2
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	6	0.2
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	9	0.2
(1,866)	1:46:A:THR:HB	1:48:A:GLU:H	4	0.2
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE1	5	0.2
(1,803)	1:177:A:ALA:HB1	1:186:A:PHE:HE2	5	0.2
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE1	5	0.2
(1,803)	1:177:A:ALA:HB2	1:186:A:PHE:HE2	5	0.2
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE1	5	0.2
(1,803)	1:177:A:ALA:HB3	1:186:A:PHE:HE2	5	0.2
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD1	9	0.2
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD2	9	0.2
(1,738)	1:119:A:TYR:HE1	1:145:A:ALA:HA	3	0.2
(1,738)	1:119:A:TYR:HE2	1:145:A:ALA:HA	3	0.2
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	3	0.2
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	3	0.2
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	3	0.2
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	3	0.2
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	3	0.2
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	3	0.2
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG21	6	0.2
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG22	6	0.2
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG23	6	0.2
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG21	7	0.2
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG22	7	0.2
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG23	7	0.2
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD11	10	0.2
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD12	10	0.2
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD13	10	0.2
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD11	10	0.2
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD12	10	0.2
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD13	10	0.2
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD11	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD12	10	0.2
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD13	10	0.2
(1,542)	1:36:A:ILE:HD11	1:40:A:ARG:HB3	10	0.2
(1,542)	1:36:A:ILE:HD12	1:40:A:ARG:HB3	10	0.2
(1,542)	1:36:A:ILE:HD13	1:40:A:ARG:HB3	10	0.2
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	5	0.2
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	5	0.2
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	5	0.2
(1,494)	1:99:A:ILE:HG21	1:151:A:THR:HB	9	0.2
(1,494)	1:99:A:ILE:HG22	1:151:A:THR:HB	9	0.2
(1,494)	1:99:A:ILE:HG23	1:151:A:THR:HB	9	0.2
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG11	8	0.2
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG12	8	0.2
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG13	8	0.2
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG11	8	0.2
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG12	8	0.2
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG13	8	0.2
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG11	8	0.2
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG12	8	0.2
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG13	8	0.2
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	7	0.2
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	7	0.2
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	7	0.2
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG21	6	0.2
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG22	6	0.2
(1,439)	1:70:A:GLU:HA	1:71:A:THR:HG23	6	0.2
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	8	0.2
(1,309)	1:118:A:MET:HE1	1:151:A:THR:HB	8	0.2
(1,309)	1:118:A:MET:HE2	1:151:A:THR:HB	8	0.2
(1,309)	1:118:A:MET:HE3	1:151:A:THR:HB	8	0.2
(1,290)	1:96:A:VAL:HG21	1:163:A:MET:HB2	2	0.2
(1,290)	1:96:A:VAL:HG22	1:163:A:MET:HB2	2	0.2
(1,290)	1:96:A:VAL:HG23	1:163:A:MET:HB2	2	0.2
(1,266)	1:180:A:LYS:HB2	1:186:A:PHE:HB2	2	0.2
(1,266)	1:180:A:LYS:HB3	1:186:A:PHE:HB2	2	0.2
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD11	8	0.2
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD12	8	0.2
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD13	8	0.2
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	2	0.2
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	2	0.2
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	2	0.2
(1,1788)	1:172:A:THR:HG21	1:191:A:CYS:HB2	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1788)	1:172:A:THR:HG21	1:191:A:CYS:HB3	3	0.19
(1,1788)	1:172:A:THR:HG22	1:191:A:CYS:HB2	3	0.19
(1,1788)	1:172:A:THR:HG22	1:191:A:CYS:HB3	3	0.19
(1,1788)	1:172:A:THR:HG23	1:191:A:CYS:HB2	3	0.19
(1,1788)	1:172:A:THR:HG23	1:191:A:CYS:HB3	3	0.19
(1,1786)	1:172:A:THR:HG21	1:175:A:TYR:HB2	1	0.19
(1,1786)	1:172:A:THR:HG21	1:175:A:TYR:HB3	1	0.19
(1,1786)	1:172:A:THR:HG22	1:175:A:TYR:HB2	1	0.19
(1,1786)	1:172:A:THR:HG22	1:175:A:TYR:HB3	1	0.19
(1,1786)	1:172:A:THR:HG23	1:175:A:TYR:HB2	1	0.19
(1,1786)	1:172:A:THR:HG23	1:175:A:TYR:HB3	1	0.19
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	6	0.19
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	6	0.19
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD11	4	0.19
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD12	4	0.19
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD13	4	0.19
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD21	4	0.19
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD22	4	0.19
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD23	4	0.19
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	2	0.19
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	2	0.19
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	2	0.19
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	2	0.19
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	2	0.19
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	2	0.19
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	5	0.19
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	5	0.19
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	5	0.19
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	5	0.19
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	5	0.19
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	5	0.19
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	5	0.19
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	5	0.19
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	5	0.19
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	5	0.19
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	5	0.19
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	5	0.19
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	5	0.19
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	5	0.19
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	5	0.19
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	5	0.19
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	5	0.19
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	5	0.19
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	5	0.19
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	5	0.19
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	5	0.19
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	5	0.19
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	5	0.19
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB2	3	0.19
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB3	3	0.19
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG11	4	0.19
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG12	4	0.19
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG13	4	0.19
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG21	4	0.19
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG22	4	0.19
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG23	4	0.19
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG11	4	0.19
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG12	4	0.19
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG13	4	0.19
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG21	4	0.19
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG22	4	0.19
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG23	4	0.19
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	4	0.19
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	4	0.19
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	4	0.19
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	4	0.19
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	4	0.19
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	4	0.19
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	4	0.19
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	4	0.19
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	4	0.19
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	4	0.19
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	4	0.19
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	4	0.19
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	4	0.19
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	4	0.19
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	4	0.19
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	4	0.19
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	4	0.19
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	4	0.19
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	10	0.19
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	10	0.19
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	10	0.19
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	10	0.19
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	10	0.19
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	5	0.19
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	5	0.19
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	5	0.19
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	5	0.19
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	5	0.19
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	5	0.19
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	5	0.19
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	5	0.19
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	5	0.19
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	5	0.19
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	5	0.19
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	5	0.19
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	10	0.19
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	10	0.19
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	10	0.19
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	10	0.19
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	10	0.19
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	10	0.19
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	10	0.19
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	10	0.19
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	10	0.19
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	10	0.19
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	10	0.19
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	10	0.19
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE1	5	0.19
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE2	5	0.19
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE3	5	0.19
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	9	0.19
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	9	0.19
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	10	0.19
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	10	0.19
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB2	5	0.19
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB3	5	0.19
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	5	0.19
(1,866)	1:46:A:THR:HB	1:48:A:GLU:H	7	0.19
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	5	0.19
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	5	0.19
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	5	0.19
(1,786)	1:66:A:PHE:HD1	1:132:A:LEU:HG	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,786)	1:66:A:PHE:HD2	1:132:A:LEU:HG	6	0.19
(1,774)	1:66:A:PHE:HD1	1:81:A:ILE:HA	6	0.19
(1,774)	1:66:A:PHE:HD2	1:81:A:ILE:HA	6	0.19
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	9	0.19
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	9	0.19
(1,738)	1:119:A:TYR:HE1	1:145:A:ALA:HA	1	0.19
(1,738)	1:119:A:TYR:HE2	1:145:A:ALA:HA	1	0.19
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	7	0.19
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	6	0.19
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	6	0.19
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	6	0.19
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	6	0.19
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	6	0.19
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	6	0.19
(1,700)	1:103:A:ALA:HB1	1:115:A:PHE:HD1	9	0.19
(1,700)	1:103:A:ALA:HB1	1:115:A:PHE:HD2	9	0.19
(1,700)	1:103:A:ALA:HB2	1:115:A:PHE:HD1	9	0.19
(1,700)	1:103:A:ALA:HB2	1:115:A:PHE:HD2	9	0.19
(1,700)	1:103:A:ALA:HB3	1:115:A:PHE:HD1	9	0.19
(1,700)	1:103:A:ALA:HB3	1:115:A:PHE:HD2	9	0.19
(1,657)	1:137:A:MET:HE1	1:140:A:THR:H	5	0.19
(1,657)	1:137:A:MET:HE2	1:140:A:THR:H	5	0.19
(1,657)	1:137:A:MET:HE3	1:140:A:THR:H	5	0.19
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	9	0.19
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	9	0.19
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	9	0.19
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	9	0.19
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	9	0.19
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	9	0.19
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	9	0.19
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	9	0.19
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	9	0.19
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD11	5	0.19
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD12	5	0.19
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD13	5	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD11	5	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD12	5	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD13	5	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD11	5	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD12	5	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD13	5	0.19
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD11	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD12	9	0.19
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD13	9	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD11	9	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD12	9	0.19
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD13	9	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD11	9	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD12	9	0.19
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD13	9	0.19
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG21	5	0.19
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG22	5	0.19
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG23	5	0.19
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	9	0.19
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE1	9	0.19
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE2	9	0.19
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE3	9	0.19
(1,309)	1:118:A:MET:HE1	1:151:A:THR:HB	6	0.19
(1,309)	1:118:A:MET:HE2	1:151:A:THR:HB	6	0.19
(1,309)	1:118:A:MET:HE3	1:151:A:THR:HB	6	0.19
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG21	1	0.19
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG22	1	0.19
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG23	1	0.19
(1,189)	1:49:A:ILE:HA	1:132:A:LEU:HG	5	0.19
(1,189)	1:49:A:ILE:HA	1:132:A:LEU:HG	7	0.19
(1,173)	1:66:A:PHE:HA	1:81:A:ILE:HD11	10	0.19
(1,173)	1:66:A:PHE:HA	1:81:A:ILE:HD12	10	0.19
(1,173)	1:66:A:PHE:HA	1:81:A:ILE:HD13	10	0.19
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	10	0.19
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	10	0.19
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	10	0.19
(1,157)	1:45:A:ILE:HG21	1:125:A:VAL:HA	5	0.19
(1,157)	1:45:A:ILE:HG22	1:125:A:VAL:HA	5	0.19
(1,157)	1:45:A:ILE:HG23	1:125:A:VAL:HA	5	0.19
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG21	3	0.19
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG22	3	0.19
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG23	3	0.19
(1,21)	1:103:A:ALA:HA	1:109:A:THR:HB	2	0.19
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE2	2	0.19
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE3	2	0.19
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	1	0.18
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	1	0.18
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG11	5	0.18
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG12	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG13	5	0.18
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG21	5	0.18
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG22	5	0.18
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG23	5	0.18
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG11	5	0.18
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG12	5	0.18
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG13	5	0.18
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG21	5	0.18
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG22	5	0.18
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG23	5	0.18
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG2	5	0.18
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG3	5	0.18
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	4	0.18
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	4	0.18
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	4	0.18
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	4	0.18
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	4	0.18
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	4	0.18
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	6	0.18
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	6	0.18
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	6	0.18
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	6	0.18
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	6	0.18
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	6	0.18
(1,1587)	1:96:A:VAL:HG11	1:164:A:LYS:H	10	0.18
(1,1587)	1:96:A:VAL:HG12	1:164:A:LYS:H	10	0.18
(1,1587)	1:96:A:VAL:HG13	1:164:A:LYS:H	10	0.18
(1,1587)	1:96:A:VAL:HG21	1:164:A:LYS:H	10	0.18
(1,1587)	1:96:A:VAL:HG22	1:164:A:LYS:H	10	0.18
(1,1587)	1:96:A:VAL:HG23	1:164:A:LYS:H	10	0.18
(1,1584)	1:96:A:VAL:HG11	1:160:A:ALA:HA	7	0.18
(1,1584)	1:96:A:VAL:HG12	1:160:A:ALA:HA	7	0.18
(1,1584)	1:96:A:VAL:HG13	1:160:A:ALA:HA	7	0.18
(1,1584)	1:96:A:VAL:HG21	1:160:A:ALA:HA	7	0.18
(1,1584)	1:96:A:VAL:HG22	1:160:A:ALA:HA	7	0.18
(1,1584)	1:96:A:VAL:HG23	1:160:A:ALA:HA	7	0.18
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB1	2	0.18
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB2	2	0.18
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB3	2	0.18
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB1	2	0.18
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB2	2	0.18
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD2	8	0.18
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD3	8	0.18
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD2	8	0.18
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD3	8	0.18
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD2	8	0.18
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD3	8	0.18
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG2	9	0.18
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG3	9	0.18
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG2	9	0.18
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG3	9	0.18
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG2	9	0.18
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG3	9	0.18
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	4	0.18
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	4	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD11	2	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD12	2	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD13	2	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD21	2	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD22	2	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD23	2	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD11	2	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD12	2	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD13	2	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD21	2	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD22	2	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD23	2	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD11	6	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD12	6	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD13	6	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD21	6	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD22	6	0.18
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD23	6	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD11	6	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD12	6	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD13	6	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD21	6	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD22	6	0.18
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD23	6	0.18
(1,1473)	1:70:A:GLU:HB2	1:71:A:THR:HA	9	0.18
(1,1473)	1:70:A:GLU:HB3	1:71:A:THR:HA	9	0.18
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	2	0.18
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	2	0.18
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	2	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	2	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	2	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	2	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	2	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	2	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	2	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	2	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	2	0.18
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	6	0.18
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	6	0.18
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	6	0.18
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	6	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	6	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	6	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	6	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	6	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	6	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	6	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	6	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	6	0.18
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	8	0.18
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	8	0.18
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	8	0.18
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	8	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	8	0.18
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	8	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	8	0.18
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	8	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	8	0.18
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	8	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	8	0.18
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	8	0.18
(1,1220)	1:149:A:PRO:HB3	1:150:A:THR:H	5	0.18
(1,1220)	1:149:A:PRO:HB3	1:150:A:THR:H	7	0.18
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	5	0.18
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	6	0.18
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	7	0.18
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB2	4	0.18
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB3	4	0.18
(1,982)	1:30:A:LEU:HD11	1:31:A:LYS:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:30:A:LEU:HD12	1:31:A:LYS:H	1	0.18
(1,982)	1:30:A:LEU:HD13	1:31:A:LYS:H	1	0.18
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	2	0.18
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	4	0.18
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	8	0.18
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE1	7	0.18
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE2	7	0.18
(1,786)	1:66:A:PHE:HD1	1:132:A:LEU:HG	9	0.18
(1,786)	1:66:A:PHE:HD2	1:132:A:LEU:HG	9	0.18
(1,778)	1:66:A:PHE:HD1	1:132:A:LEU:HB2	6	0.18
(1,778)	1:66:A:PHE:HD2	1:132:A:LEU:HB2	6	0.18
(1,774)	1:66:A:PHE:HD1	1:81:A:ILE:HA	10	0.18
(1,774)	1:66:A:PHE:HD2	1:81:A:ILE:HA	10	0.18
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD1	7	0.18
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD2	7	0.18
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	1	0.18
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	1	0.18
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	5	0.18
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	5	0.18
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	5	0.18
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD11	7	0.18
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD12	7	0.18
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD13	7	0.18
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	9	0.18
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	9	0.18
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD21	4	0.18
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD22	4	0.18
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD23	4	0.18
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD21	4	0.18
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD22	4	0.18
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD23	4	0.18
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD21	4	0.18
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD22	4	0.18
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD23	4	0.18
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	1	0.18
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	4	0.18
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	7	0.18
(1,477)	1:103:A:ALA:HB1	1:153:A:ALA:HB1	4	0.18
(1,477)	1:103:A:ALA:HB1	1:153:A:ALA:HB2	4	0.18
(1,477)	1:103:A:ALA:HB1	1:153:A:ALA:HB3	4	0.18
(1,477)	1:103:A:ALA:HB2	1:153:A:ALA:HB1	4	0.18
(1,477)	1:103:A:ALA:HB2	1:153:A:ALA:HB2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:103:A:ALA:HB2	1:153:A:ALA:HB3	4	0.18
(1,477)	1:103:A:ALA:HB3	1:153:A:ALA:HB1	4	0.18
(1,477)	1:103:A:ALA:HB3	1:153:A:ALA:HB2	4	0.18
(1,477)	1:103:A:ALA:HB3	1:153:A:ALA:HB3	4	0.18
(1,447)	1:97:A:THR:HG21	1:101:A:GLY:HA2	1	0.18
(1,447)	1:97:A:THR:HG22	1:101:A:GLY:HA2	1	0.18
(1,447)	1:97:A:THR:HG23	1:101:A:GLY:HA2	1	0.18
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG21	2	0.18
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG22	2	0.18
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG23	2	0.18
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	5	0.18
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	5	0.18
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	5	0.18
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	5	0.18
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	5	0.18
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	5	0.18
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	5	0.18
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	5	0.18
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	5	0.18
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	8	0.18
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	8	0.18
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	8	0.18
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	8	0.18
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	8	0.18
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	8	0.18
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	8	0.18
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	8	0.18
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	8	0.18
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG12	8	0.18
(1,399)	1:149:A:PRO:HG3	1:159:A:ILE:HG13	8	0.18
(1,326)	1:107:A:LYS:HB2	1:108:A:LYS:HE2	8	0.18
(1,326)	1:107:A:LYS:HB2	1:108:A:LYS:HE3	8	0.18
(1,326)	1:107:A:LYS:HB3	1:108:A:LYS:HE2	8	0.18
(1,326)	1:107:A:LYS:HB3	1:108:A:LYS:HE3	8	0.18
(1,309)	1:118:A:MET:HE1	1:151:A:THR:HB	4	0.18
(1,309)	1:118:A:MET:HE2	1:151:A:THR:HB	4	0.18
(1,309)	1:118:A:MET:HE3	1:151:A:THR:HB	4	0.18
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	6	0.18
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	9	0.18
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	9	0.18
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	9	0.18
(1,76)	1:63:A:PHE:HA	1:81:A:ILE:HG21	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:63:A:PHE:HA	1:81:A:ILE:HG22	10	0.18
(1,76)	1:63:A:PHE:HA	1:81:A:ILE:HG23	10	0.18
(1,1753)	1:154:A:GLU:HG2	1:157:A:LEU:HD11	1	0.17
(1,1753)	1:154:A:GLU:HG2	1:157:A:LEU:HD12	1	0.17
(1,1753)	1:154:A:GLU:HG2	1:157:A:LEU:HD13	1	0.17
(1,1753)	1:154:A:GLU:HG2	1:157:A:LEU:HD21	1	0.17
(1,1753)	1:154:A:GLU:HG2	1:157:A:LEU:HD22	1	0.17
(1,1753)	1:154:A:GLU:HG2	1:157:A:LEU:HD23	1	0.17
(1,1753)	1:154:A:GLU:HG3	1:157:A:LEU:HD11	1	0.17
(1,1753)	1:154:A:GLU:HG3	1:157:A:LEU:HD12	1	0.17
(1,1753)	1:154:A:GLU:HG3	1:157:A:LEU:HD13	1	0.17
(1,1753)	1:154:A:GLU:HG3	1:157:A:LEU:HD21	1	0.17
(1,1753)	1:154:A:GLU:HG3	1:157:A:LEU:HD22	1	0.17
(1,1753)	1:154:A:GLU:HG3	1:157:A:LEU:HD23	1	0.17
(1,1719)	1:141:A:VAL:HG11	1:162:A:ILE:HB	1	0.17
(1,1719)	1:141:A:VAL:HG12	1:162:A:ILE:HB	1	0.17
(1,1719)	1:141:A:VAL:HG13	1:162:A:ILE:HB	1	0.17
(1,1719)	1:141:A:VAL:HG21	1:162:A:ILE:HB	1	0.17
(1,1719)	1:141:A:VAL:HG22	1:162:A:ILE:HB	1	0.17
(1,1719)	1:141:A:VAL:HG23	1:162:A:ILE:HB	1	0.17
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG12	2	0.17
(1,1620)	1:103:A:ALA:HA	1:156:A:ILE:HG13	2	0.17
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	4	0.17
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	4	0.17
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	4	0.17
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	4	0.17
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	4	0.17
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	4	0.17
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	9	0.17
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	9	0.17
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	9	0.17
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	9	0.17
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	9	0.17
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	9	0.17
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG2	1	0.17
(1,1525)	1:84:A:ALA:HB1	1:87:A:ARG:HG3	1	0.17
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG2	1	0.17
(1,1525)	1:84:A:ALA:HB2	1:87:A:ARG:HG3	1	0.17
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG2	1	0.17
(1,1525)	1:84:A:ALA:HB3	1:87:A:ARG:HG3	1	0.17
(1,1523)	1:84:A:ALA:H	1:178:A:LEU:HD11	2	0.17
(1,1523)	1:84:A:ALA:H	1:178:A:LEU:HD12	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1523)	1:84:A:ALA:H	1:178:A:LEU:HD13	2	0.17
(1,1523)	1:84:A:ALA:H	1:178:A:LEU:HD21	2	0.17
(1,1523)	1:84:A:ALA:H	1:178:A:LEU:HD22	2	0.17
(1,1523)	1:84:A:ALA:H	1:178:A:LEU:HD23	2	0.17
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD11	1	0.17
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD12	1	0.17
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD13	1	0.17
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD11	1	0.17
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD12	1	0.17
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD13	1	0.17
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG11	1	0.17
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG12	1	0.17
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG13	1	0.17
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG21	1	0.17
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG22	1	0.17
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG23	1	0.17
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG11	1	0.17
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG12	1	0.17
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG13	1	0.17
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG21	1	0.17
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG22	1	0.17
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG23	1	0.17
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	2	0.17
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	2	0.17
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	2	0.17
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	2	0.17
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	2	0.17
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	2	0.17
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	2	0.17
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	2	0.17
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	2	0.17
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	2	0.17
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	2	0.17
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	2	0.17
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	2	0.17
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	2	0.17
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	2	0.17
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	2	0.17
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	2	0.17
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	2	0.17
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	10	0.17
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG12	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG13	3	0.17
(1,1060)	1:177:A:ALA:HB1	1:181:A:LYS:H	1	0.17
(1,1060)	1:177:A:ALA:HB2	1:181:A:LYS:H	1	0.17
(1,1060)	1:177:A:ALA:HB3	1:181:A:LYS:H	1	0.17
(1,969)	1:160:A:ALA:H	1:161:A:LYS:HB3	10	0.17
(1,802)	1:66:A:PHE:HE1	1:81:A:ILE:HB	7	0.17
(1,802)	1:66:A:PHE:HE2	1:81:A:ILE:HB	7	0.17
(1,774)	1:66:A:PHE:HD1	1:81:A:ILE:HA	1	0.17
(1,774)	1:66:A:PHE:HD2	1:81:A:ILE:HA	1	0.17
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD1	10	0.17
(1,771)	1:113:A:GLY:HA3	1:115:A:PHE:HD2	10	0.17
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD11	5	0.17
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD12	5	0.17
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD13	5	0.17
(1,588)	1:145:A:ALA:HA	1:150:A:THR:HG21	8	0.17
(1,588)	1:145:A:ALA:HA	1:150:A:THR:HG22	8	0.17
(1,588)	1:145:A:ALA:HA	1:150:A:THR:HG23	8	0.17
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD11	5	0.17
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD12	5	0.17
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD13	5	0.17
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD11	5	0.17
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD12	5	0.17
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD13	5	0.17
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD11	5	0.17
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD12	5	0.17
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD13	5	0.17
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	2	0.17
(1,492)	1:97:A:THR:HB	1:167:A:LEU:HG	5	0.17
(1,492)	1:97:A:THR:HB	1:167:A:LEU:HG	7	0.17
(1,480)	1:140:A:THR:HG21	1:162:A:ILE:HG21	1	0.17
(1,480)	1:140:A:THR:HG21	1:162:A:ILE:HG22	1	0.17
(1,480)	1:140:A:THR:HG21	1:162:A:ILE:HG23	1	0.17
(1,480)	1:140:A:THR:HG22	1:162:A:ILE:HG21	1	0.17
(1,480)	1:140:A:THR:HG22	1:162:A:ILE:HG22	1	0.17
(1,480)	1:140:A:THR:HG22	1:162:A:ILE:HG23	1	0.17
(1,480)	1:140:A:THR:HG23	1:162:A:ILE:HG21	1	0.17
(1,480)	1:140:A:THR:HG23	1:162:A:ILE:HG22	1	0.17
(1,480)	1:140:A:THR:HG23	1:162:A:ILE:HG23	1	0.17
(1,419)	1:49:A:ILE:HG21	1:132:A:LEU:HB3	7	0.17
(1,419)	1:49:A:ILE:HG22	1:132:A:LEU:HB3	7	0.17
(1,419)	1:49:A:ILE:HG23	1:132:A:LEU:HB3	7	0.17
(1,305)	1:149:A:PRO:HB3	1:152:A:THR:HB	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:149:A:PRO:HB3	1:152:A:THR:HB	6	0.17
(1,123)	1:83:A:GLU:HA	1:86:A:VAL:HG11	8	0.17
(1,123)	1:83:A:GLU:HA	1:86:A:VAL:HG12	8	0.17
(1,123)	1:83:A:GLU:HA	1:86:A:VAL:HG13	8	0.17
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB1	8	0.17
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB2	8	0.17
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB3	8	0.17
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG11	4	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG12	4	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG13	4	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG21	4	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG22	4	0.16
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG23	4	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG11	4	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG12	4	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG13	4	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG21	4	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG22	4	0.16
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG23	4	0.16
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE1	5	0.16
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE2	5	0.16
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE3	5	0.16
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE1	5	0.16
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE2	5	0.16
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE3	5	0.16
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	6	0.16
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	6	0.16
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	6	0.16
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	6	0.16
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	6	0.16
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	6	0.16
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	1	0.16
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	1	0.16
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG11	3	0.16
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG12	3	0.16
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG13	3	0.16
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG21	3	0.16
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG22	3	0.16
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG23	3	0.16
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG11	3	0.16
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG12	3	0.16
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG13	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG21	3	0.16
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG22	3	0.16
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG23	3	0.16
(1,1331)	1:30:A:LEU:HD11	1:34:A:THR:H	2	0.16
(1,1331)	1:30:A:LEU:HD12	1:34:A:THR:H	2	0.16
(1,1331)	1:30:A:LEU:HD13	1:34:A:THR:H	2	0.16
(1,1331)	1:30:A:LEU:HD21	1:34:A:THR:H	2	0.16
(1,1331)	1:30:A:LEU:HD22	1:34:A:THR:H	2	0.16
(1,1331)	1:30:A:LEU:HD23	1:34:A:THR:H	2	0.16
(1,1331)	1:30:A:LEU:HD11	1:34:A:THR:H	8	0.16
(1,1331)	1:30:A:LEU:HD12	1:34:A:THR:H	8	0.16
(1,1331)	1:30:A:LEU:HD13	1:34:A:THR:H	8	0.16
(1,1331)	1:30:A:LEU:HD21	1:34:A:THR:H	8	0.16
(1,1331)	1:30:A:LEU:HD22	1:34:A:THR:H	8	0.16
(1,1331)	1:30:A:LEU:HD23	1:34:A:THR:H	8	0.16
(1,1315)	1:29:A:GLY:HA2	1:30:A:LEU:HD11	9	0.16
(1,1315)	1:29:A:GLY:HA2	1:30:A:LEU:HD12	9	0.16
(1,1315)	1:29:A:GLY:HA2	1:30:A:LEU:HD13	9	0.16
(1,1315)	1:29:A:GLY:HA2	1:30:A:LEU:HD21	9	0.16
(1,1315)	1:29:A:GLY:HA2	1:30:A:LEU:HD22	9	0.16
(1,1315)	1:29:A:GLY:HA2	1:30:A:LEU:HD23	9	0.16
(1,1315)	1:29:A:GLY:HA3	1:30:A:LEU:HD11	9	0.16
(1,1315)	1:29:A:GLY:HA3	1:30:A:LEU:HD12	9	0.16
(1,1315)	1:29:A:GLY:HA3	1:30:A:LEU:HD13	9	0.16
(1,1315)	1:29:A:GLY:HA3	1:30:A:LEU:HD21	9	0.16
(1,1315)	1:29:A:GLY:HA3	1:30:A:LEU:HD22	9	0.16
(1,1315)	1:29:A:GLY:HA3	1:30:A:LEU:HD23	9	0.16
(1,1268)	1:152:A:THR:H	1:153:A:ALA:HB1	9	0.16
(1,1268)	1:152:A:THR:H	1:153:A:ALA:HB2	9	0.16
(1,1268)	1:152:A:THR:H	1:153:A:ALA:HB3	9	0.16
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	2	0.16
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG12	4	0.16
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG13	4	0.16
(1,1018)	1:116:A:SER:HB2	1:118:A:MET:H	1	0.16
(1,1018)	1:116:A:SER:HB3	1:118:A:MET:H	1	0.16
(1,1018)	1:116:A:SER:HB2	1:118:A:MET:H	5	0.16
(1,1018)	1:116:A:SER:HB3	1:118:A:MET:H	5	0.16
(1,1018)	1:116:A:SER:HB2	1:118:A:MET:H	8	0.16
(1,1018)	1:116:A:SER:HB3	1:118:A:MET:H	8	0.16
(1,795)	1:66:A:PHE:HE1	1:132:A:LEU:HA	2	0.16
(1,795)	1:66:A:PHE:HE2	1:132:A:LEU:HA	2	0.16
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE1	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE2	3	0.16
(1,786)	1:66:A:PHE:HD1	1:132:A:LEU:HG	2	0.16
(1,786)	1:66:A:PHE:HD2	1:132:A:LEU:HG	2	0.16
(1,786)	1:66:A:PHE:HD1	1:132:A:LEU:HG	8	0.16
(1,786)	1:66:A:PHE:HD2	1:132:A:LEU:HG	8	0.16
(1,774)	1:66:A:PHE:HD1	1:81:A:ILE:HA	7	0.16
(1,774)	1:66:A:PHE:HD2	1:81:A:ILE:HA	7	0.16
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	7	0.16
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	7	0.16
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	8	0.16
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	7	0.16
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	7	0.16
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	7	0.16
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	7	0.16
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	7	0.16
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	7	0.16
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG21	5	0.16
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG22	5	0.16
(1,702)	1:80:A:PHE:HZ	1:81:A:ILE:HG23	5	0.16
(1,687)	1:55:A:ASP:HA	1:80:A:PHE:HZ	3	0.16
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	1	0.16
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	1	0.16
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	5	0.16
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	5	0.16
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	6	0.16
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	6	0.16
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	6	0.16
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	6	0.16
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	6	0.16
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	6	0.16
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	6	0.16
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	6	0.16
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	6	0.16
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	2	0.16
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	2	0.16
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	2	0.16
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD21	10	0.16
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD22	10	0.16
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD23	10	0.16
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD21	10	0.16
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD22	10	0.16
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD23	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD21	10	0.16
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD22	10	0.16
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD23	10	0.16
(1,524)	1:42:A:ALA:HA	1:45:A:ILE:HD11	7	0.16
(1,524)	1:42:A:ALA:HA	1:45:A:ILE:HD12	7	0.16
(1,524)	1:42:A:ALA:HA	1:45:A:ILE:HD13	7	0.16
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG21	6	0.16
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG22	6	0.16
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG23	6	0.16
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	6	0.16
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	6	0.16
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	6	0.16
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	6	0.16
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	6	0.16
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	6	0.16
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	6	0.16
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	6	0.16
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	6	0.16
(1,400)	1:92:A:ALA:HB1	1:129:A:LEU:HG	8	0.16
(1,400)	1:92:A:ALA:HB2	1:129:A:LEU:HG	8	0.16
(1,400)	1:92:A:ALA:HB3	1:129:A:LEU:HG	8	0.16
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	5	0.16
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	9	0.16
(1,248)	1:96:A:VAL:HA	1:99:A:ILE:HG21	8	0.16
(1,248)	1:96:A:VAL:HA	1:99:A:ILE:HG22	8	0.16
(1,248)	1:96:A:VAL:HA	1:99:A:ILE:HG23	8	0.16
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	7	0.16
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	7	0.16
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	7	0.16
(1,121)	1:89:A:THR:HG21	1:171:A:HIS:HA	10	0.16
(1,121)	1:89:A:THR:HG22	1:171:A:HIS:HA	10	0.16
(1,121)	1:89:A:THR:HG23	1:171:A:HIS:HA	10	0.16
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE2	10	0.16
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE3	10	0.16
(1,21)	1:103:A:ALA:HA	1:109:A:THR:HB	6	0.16
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA2	2	0.15
(1,1737)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	2	0.15
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG11	9	0.15
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG12	9	0.15
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG13	9	0.15
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG21	9	0.15
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG22	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1699)	1:130:A:GLU:HG2	1:134:A:VAL:HG23	9	0.15
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG11	9	0.15
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG12	9	0.15
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG13	9	0.15
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG21	9	0.15
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG22	9	0.15
(1,1699)	1:130:A:GLU:HG3	1:134:A:VAL:HG23	9	0.15
(1,1670)	1:123:A:LEU:HD11	1:141:A:VAL:HB	2	0.15
(1,1670)	1:123:A:LEU:HD12	1:141:A:VAL:HB	2	0.15
(1,1670)	1:123:A:LEU:HD13	1:141:A:VAL:HB	2	0.15
(1,1670)	1:123:A:LEU:HD21	1:141:A:VAL:HB	2	0.15
(1,1670)	1:123:A:LEU:HD22	1:141:A:VAL:HB	2	0.15
(1,1670)	1:123:A:LEU:HD23	1:141:A:VAL:HB	2	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD11	7	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD12	7	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD13	7	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD21	7	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD22	7	0.15
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD23	7	0.15
(1,1650)	1:115:A:PHE:HB2	1:118:A:MET:HE1	7	0.15
(1,1650)	1:115:A:PHE:HB2	1:118:A:MET:HE2	7	0.15
(1,1650)	1:115:A:PHE:HB2	1:118:A:MET:HE3	7	0.15
(1,1650)	1:115:A:PHE:HB3	1:118:A:MET:HE1	7	0.15
(1,1650)	1:115:A:PHE:HB3	1:118:A:MET:HE2	7	0.15
(1,1650)	1:115:A:PHE:HB3	1:118:A:MET:HE3	7	0.15
(1,1639)	1:108:A:LYS:HA	1:108:A:LYS:HD2	5	0.15
(1,1639)	1:108:A:LYS:HA	1:108:A:LYS:HD3	5	0.15
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG2	6	0.15
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG3	6	0.15
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE2	2	0.15
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE3	2	0.15
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE2	2	0.15
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE3	2	0.15
(1,1506)	1:82:A:LEU:HD11	1:174:A:ASN:HA	5	0.15
(1,1506)	1:82:A:LEU:HD12	1:174:A:ASN:HA	5	0.15
(1,1506)	1:82:A:LEU:HD13	1:174:A:ASN:HA	5	0.15
(1,1506)	1:82:A:LEU:HD21	1:174:A:ASN:HA	5	0.15
(1,1506)	1:82:A:LEU:HD22	1:174:A:ASN:HA	5	0.15
(1,1506)	1:82:A:LEU:HD23	1:174:A:ASN:HA	5	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	3	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	3	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	3	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	3	0.15
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	3	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	3	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	3	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	3	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	3	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	3	0.15
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	3	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	3	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	3	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	3	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	3	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	3	0.15
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	3	0.15
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	1	0.15
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	1	0.15
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	1	0.15
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	1	0.15
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	1	0.15
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	1	0.15
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	5	0.15
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	5	0.15
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	5	0.15
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	5	0.15
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	5	0.15
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	5	0.15
(1,1162)	1:109:A:THR:HB	1:116:A:SER:H	7	0.15
(1,1137)	1:172:A:THR:HG21	1:174:A:ASN:H	6	0.15
(1,1137)	1:172:A:THR:HG22	1:174:A:ASN:H	6	0.15
(1,1137)	1:172:A:THR:HG23	1:174:A:ASN:H	6	0.15
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	3	0.15
(1,1018)	1:116:A:SER:HB2	1:118:A:MET:H	6	0.15
(1,1018)	1:116:A:SER:HB3	1:118:A:MET:H	6	0.15
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	4	0.15
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	4	0.15
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	4	0.15
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	7	0.15
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	7	0.15
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	7	0.15
(1,795)	1:66:A:PHE:HE1	1:132:A:LEU:HA	7	0.15
(1,795)	1:66:A:PHE:HE2	1:132:A:LEU:HA	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:66:A:PHE:HE1	1:132:A:LEU:HA	9	0.15
(1,795)	1:66:A:PHE:HE2	1:132:A:LEU:HA	9	0.15
(1,693)	1:86:A:VAL:HG11	1:171:A:HIS:HD2	2	0.15
(1,693)	1:86:A:VAL:HG12	1:171:A:HIS:HD2	2	0.15
(1,693)	1:86:A:VAL:HG13	1:171:A:HIS:HD2	2	0.15
(1,687)	1:55:A:ASP:HA	1:80:A:PHE:HZ	6	0.15
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD11	3	0.15
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD12	3	0.15
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD13	3	0.15
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD11	6	0.15
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD12	6	0.15
(1,640)	1:119:A:TYR:H	1:156:A:ILE:HD13	6	0.15
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG21	7	0.15
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG22	7	0.15
(1,597)	1:150:A:THR:HG21	1:159:A:ILE:HG23	7	0.15
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG21	7	0.15
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG22	7	0.15
(1,597)	1:150:A:THR:HG22	1:159:A:ILE:HG23	7	0.15
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG21	7	0.15
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG22	7	0.15
(1,597)	1:150:A:THR:HG23	1:159:A:ILE:HG23	7	0.15
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	9	0.15
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	9	0.15
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	9	0.15
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	10	0.15
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	10	0.15
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	10	0.15
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD11	6	0.15
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD12	6	0.15
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD13	6	0.15
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD11	6	0.15
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD12	6	0.15
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD13	6	0.15
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD11	6	0.15
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD12	6	0.15
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD13	6	0.15
(1,568)	1:153:A:ALA:HB1	1:157:A:LEU:HD21	10	0.15
(1,568)	1:153:A:ALA:HB1	1:157:A:LEU:HD22	10	0.15
(1,568)	1:153:A:ALA:HB1	1:157:A:LEU:HD23	10	0.15
(1,568)	1:153:A:ALA:HB2	1:157:A:LEU:HD21	10	0.15
(1,568)	1:153:A:ALA:HB2	1:157:A:LEU:HD22	10	0.15
(1,568)	1:153:A:ALA:HB2	1:157:A:LEU:HD23	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:153:A:ALA:HB3	1:157:A:LEU:HD21	10	0.15
(1,568)	1:153:A:ALA:HB3	1:157:A:LEU:HD22	10	0.15
(1,568)	1:153:A:ALA:HB3	1:157:A:LEU:HD23	10	0.15
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB1	4	0.15
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB2	4	0.15
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB3	4	0.15
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB1	4	0.15
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB2	4	0.15
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB3	4	0.15
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB1	4	0.15
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB2	4	0.15
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB3	4	0.15
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	3	0.15
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	3	0.15
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	3	0.15
(1,506)	1:164:A:LYS:HA	1:167:A:LEU:HG	10	0.15
(1,396)	1:103:A:ALA:HB1	1:115:A:PHE:HB2	7	0.15
(1,396)	1:103:A:ALA:HB1	1:115:A:PHE:HB3	7	0.15
(1,396)	1:103:A:ALA:HB2	1:115:A:PHE:HB2	7	0.15
(1,396)	1:103:A:ALA:HB2	1:115:A:PHE:HB3	7	0.15
(1,396)	1:103:A:ALA:HB3	1:115:A:PHE:HB2	7	0.15
(1,396)	1:103:A:ALA:HB3	1:115:A:PHE:HB3	7	0.15
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB1	7	0.15
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB2	7	0.15
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB3	7	0.15
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	2	0.15
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	5	0.15
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD11	9	0.15
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD12	9	0.15
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD13	9	0.15
(1,200)	1:137:A:MET:HE1	1:141:A:VAL:HA	2	0.15
(1,200)	1:137:A:MET:HE2	1:141:A:VAL:HA	2	0.15
(1,200)	1:137:A:MET:HE3	1:141:A:VAL:HA	2	0.15
(1,157)	1:45:A:ILE:HG21	1:125:A:VAL:HA	3	0.15
(1,157)	1:45:A:ILE:HG22	1:125:A:VAL:HA	3	0.15
(1,157)	1:45:A:ILE:HG23	1:125:A:VAL:HA	3	0.15
(1,98)	1:33:A:GLU:HA	1:36:A:ILE:HB	5	0.15
(1,73)	1:144:A:ALA:HA	1:162:A:ILE:HG21	10	0.15
(1,73)	1:144:A:ALA:HA	1:162:A:ILE:HG22	10	0.15
(1,73)	1:144:A:ALA:HA	1:162:A:ILE:HG23	10	0.15
(1,21)	1:103:A:ALA:HA	1:109:A:THR:HB	3	0.15
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE1	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	1:178:A:LEU:HB2	1:186:A:PHE:HE2	9	0.14
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE1	9	0.14
(1,1805)	1:178:A:LEU:HB3	1:186:A:PHE:HE2	9	0.14
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG2	7	0.14
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG3	7	0.14
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE1	1	0.14
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE2	1	0.14
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE3	1	0.14
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE1	1	0.14
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE2	1	0.14
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE3	1	0.14
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB1	4	0.14
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB2	4	0.14
(1,1548)	1:87:A:ARG:HG2	1:88:A:ALA:HB3	4	0.14
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB1	4	0.14
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB2	4	0.14
(1,1548)	1:87:A:ARG:HG3	1:88:A:ALA:HB3	4	0.14
(1,1506)	1:82:A:LEU:HD11	1:174:A:ASN:HA	4	0.14
(1,1506)	1:82:A:LEU:HD12	1:174:A:ASN:HA	4	0.14
(1,1506)	1:82:A:LEU:HD13	1:174:A:ASN:HA	4	0.14
(1,1506)	1:82:A:LEU:HD21	1:174:A:ASN:HA	4	0.14
(1,1506)	1:82:A:LEU:HD22	1:174:A:ASN:HA	4	0.14
(1,1506)	1:82:A:LEU:HD23	1:174:A:ASN:HA	4	0.14
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	1	0.14
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	1	0.14
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	1	0.14
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	1	0.14
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	1	0.14
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	1	0.14
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	1	0.14
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	1	0.14
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	1	0.14
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	1	0.14
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	1	0.14
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	1	0.14
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	1	0.14
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	1	0.14
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	1	0.14
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	1	0.14
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	1	0.14
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	1	0.14
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	5	0.14
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD11	9	0.14
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD12	9	0.14
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD13	9	0.14
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD21	9	0.14
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD22	9	0.14
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD23	9	0.14
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD11	9	0.14
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD12	9	0.14
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD13	9	0.14
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD21	9	0.14
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD22	9	0.14
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD23	9	0.14
(1,1477)	1:75:A:VAL:HG11	1:77:A:GLU:HA	4	0.14
(1,1477)	1:75:A:VAL:HG12	1:77:A:GLU:HA	4	0.14
(1,1477)	1:75:A:VAL:HG13	1:77:A:GLU:HA	4	0.14
(1,1477)	1:75:A:VAL:HG21	1:77:A:GLU:HA	4	0.14
(1,1477)	1:75:A:VAL:HG22	1:77:A:GLU:HA	4	0.14
(1,1477)	1:75:A:VAL:HG23	1:77:A:GLU:HA	4	0.14
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD11	2	0.14
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD12	2	0.14
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD13	2	0.14
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD11	2	0.14
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD12	2	0.14
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD13	2	0.14
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG11	5	0.14
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG12	5	0.14
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG13	5	0.14
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG21	5	0.14
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG22	5	0.14
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG23	5	0.14
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG11	5	0.14
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG12	5	0.14
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG13	5	0.14
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG21	5	0.14
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG22	5	0.14
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG23	5	0.14
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	2	0.14
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	2	0.14
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	2	0.14
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	2	0.14
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	2	0.14
(1,1331)	1:30:A:LEU:HD11	1:34:A:THR:H	4	0.14
(1,1331)	1:30:A:LEU:HD12	1:34:A:THR:H	4	0.14
(1,1331)	1:30:A:LEU:HD13	1:34:A:THR:H	4	0.14
(1,1331)	1:30:A:LEU:HD21	1:34:A:THR:H	4	0.14
(1,1331)	1:30:A:LEU:HD22	1:34:A:THR:H	4	0.14
(1,1331)	1:30:A:LEU:HD23	1:34:A:THR:H	4	0.14
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	4	0.14
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	9	0.14
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB2	1	0.14
(1,1042)	1:49:A:ILE:H	1:51:A:LYS:HB3	1	0.14
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE1	5	0.14
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE2	5	0.14
(1,755)	1:175:A:TYR:HD1	1:179:A:GLU:HA	2	0.14
(1,755)	1:175:A:TYR:HD2	1:179:A:GLU:HA	2	0.14
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	4	0.14
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	4	0.14
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG21	6	0.14
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG22	6	0.14
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG23	6	0.14
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD11	10	0.14
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD12	10	0.14
(1,717)	1:119:A:TYR:HE1	1:159:A:ILE:HD13	10	0.14
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD11	10	0.14
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD12	10	0.14
(1,717)	1:119:A:TYR:HE2	1:159:A:ILE:HD13	10	0.14
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	7	0.14
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	7	0.14
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	8	0.14
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	8	0.14
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	4	0.14
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	4	0.14
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	4	0.14
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD21	8	0.14
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD22	8	0.14
(1,574)	1:81:A:ILE:HG21	1:82:A:LEU:HD23	8	0.14
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD21	8	0.14
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD22	8	0.14
(1,574)	1:81:A:ILE:HG22	1:82:A:LEU:HD23	8	0.14
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD21	8	0.14
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD22	8	0.14
(1,574)	1:81:A:ILE:HG23	1:82:A:LEU:HD23	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE1	8	0.14
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE2	8	0.14
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE3	8	0.14
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE1	8	0.14
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE2	8	0.14
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE3	8	0.14
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE1	8	0.14
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE2	8	0.14
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE3	8	0.14
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	6	0.14
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	6	0.14
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	6	0.14
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	9	0.14
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	9	0.14
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	9	0.14
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG11	6	0.14
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG12	6	0.14
(1,481)	1:45:A:ILE:HG21	1:91:A:VAL:HG13	6	0.14
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG11	6	0.14
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG12	6	0.14
(1,481)	1:45:A:ILE:HG22	1:91:A:VAL:HG13	6	0.14
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG11	6	0.14
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG12	6	0.14
(1,481)	1:45:A:ILE:HG23	1:91:A:VAL:HG13	6	0.14
(1,466)	1:88:A:ALA:HB1	1:132:A:LEU:HG	3	0.14
(1,466)	1:88:A:ALA:HB2	1:132:A:LEU:HG	3	0.14
(1,466)	1:88:A:ALA:HB3	1:132:A:LEU:HG	3	0.14
(1,462)	1:37:A:ILE:HG12	1:40:A:ARG:HB3	4	0.14
(1,462)	1:37:A:ILE:HG13	1:40:A:ARG:HB3	4	0.14
(1,430)	1:138:A:THR:HB	1:142:A:THR:HG21	9	0.14
(1,430)	1:138:A:THR:HB	1:142:A:THR:HG22	9	0.14
(1,430)	1:138:A:THR:HB	1:142:A:THR:HG23	9	0.14
(1,419)	1:49:A:ILE:HG21	1:132:A:LEU:HB3	8	0.14
(1,419)	1:49:A:ILE:HG22	1:132:A:LEU:HB3	8	0.14
(1,419)	1:49:A:ILE:HG23	1:132:A:LEU:HB3	8	0.14
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	3	0.14
(1,389)	1:88:A:ALA:HA	1:132:A:LEU:HB2	4	0.14
(1,257)	1:148:A:HIS:HB3	1:150:A:THR:HA	3	0.14
(1,229)	1:83:A:GLU:HG3	1:87:A:ARG:HD3	5	0.14
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE1	9	0.14
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE2	9	0.14
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE1	10	0.14
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE2	10	0.14
(1,207)	1:42:A:ALA:HA	1:121:A:MET:HE3	10	0.14
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE1	5	0.14
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE2	5	0.14
(1,202)	1:119:A:TYR:HB3	1:163:A:MET:HE3	5	0.14
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	8	0.14
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	8	0.14
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	8	0.14
(1,158)	1:99:A:ILE:HG21	1:160:A:ALA:HA	7	0.14
(1,158)	1:99:A:ILE:HG22	1:160:A:ALA:HA	7	0.14
(1,158)	1:99:A:ILE:HG23	1:160:A:ALA:HA	7	0.14
(1,157)	1:45:A:ILE:HG21	1:125:A:VAL:HA	2	0.14
(1,157)	1:45:A:ILE:HG22	1:125:A:VAL:HA	2	0.14
(1,157)	1:45:A:ILE:HG23	1:125:A:VAL:HA	2	0.14
(1,97)	1:175:A:TYR:HA	1:176:A:CYS:HB2	1	0.14
(1,97)	1:175:A:TYR:HA	1:176:A:CYS:HB3	1	0.14
(1,49)	1:30:A:LEU:HG	1:34:A:THR:HB	10	0.14
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE2	4	0.14
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE3	4	0.14
(1,1788)	1:172:A:THR:HG21	1:191:A:CYS:HB2	2	0.13
(1,1788)	1:172:A:THR:HG21	1:191:A:CYS:HB3	2	0.13
(1,1788)	1:172:A:THR:HG22	1:191:A:CYS:HB2	2	0.13
(1,1788)	1:172:A:THR:HG22	1:191:A:CYS:HB3	2	0.13
(1,1788)	1:172:A:THR:HG23	1:191:A:CYS:HB2	2	0.13
(1,1788)	1:172:A:THR:HG23	1:191:A:CYS:HB3	2	0.13
(1,1785)	1:172:A:THR:HB	1:190:A:LYS:HB2	6	0.13
(1,1785)	1:172:A:THR:HB	1:190:A:LYS:HB3	6	0.13
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG2	10	0.13
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG3	10	0.13
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG2	8	0.13
(1,1626)	1:105:A:LYS:H	1:108:A:LYS:HG3	8	0.13
(1,1584)	1:96:A:VAL:HG11	1:160:A:ALA:HA	2	0.13
(1,1584)	1:96:A:VAL:HG12	1:160:A:ALA:HA	2	0.13
(1,1584)	1:96:A:VAL:HG13	1:160:A:ALA:HA	2	0.13
(1,1584)	1:96:A:VAL:HG21	1:160:A:ALA:HA	2	0.13
(1,1584)	1:96:A:VAL:HG22	1:160:A:ALA:HA	2	0.13
(1,1584)	1:96:A:VAL:HG23	1:160:A:ALA:HA	2	0.13
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD2	3	0.13
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD3	3	0.13
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD2	3	0.13
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD2	3	0.13
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD3	3	0.13
(1,1506)	1:82:A:LEU:HD11	1:174:A:ASN:HA	7	0.13
(1,1506)	1:82:A:LEU:HD12	1:174:A:ASN:HA	7	0.13
(1,1506)	1:82:A:LEU:HD13	1:174:A:ASN:HA	7	0.13
(1,1506)	1:82:A:LEU:HD21	1:174:A:ASN:HA	7	0.13
(1,1506)	1:82:A:LEU:HD22	1:174:A:ASN:HA	7	0.13
(1,1506)	1:82:A:LEU:HD23	1:174:A:ASN:HA	7	0.13
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	6	0.13
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	6	0.13
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	6	0.13
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	6	0.13
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	6	0.13
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	6	0.13
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	6	0.13
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	6	0.13
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	6	0.13
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	6	0.13
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	6	0.13
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	6	0.13
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	6	0.13
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	6	0.13
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	6	0.13
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	6	0.13
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	6	0.13
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	6	0.13
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG12	6	0.13
(1,1495)	1:80:A:PHE:HZ	1:81:A:ILE:HG13	6	0.13
(1,1477)	1:75:A:VAL:HG11	1:77:A:GLU:HA	8	0.13
(1,1477)	1:75:A:VAL:HG12	1:77:A:GLU:HA	8	0.13
(1,1477)	1:75:A:VAL:HG13	1:77:A:GLU:HA	8	0.13
(1,1477)	1:75:A:VAL:HG21	1:77:A:GLU:HA	8	0.13
(1,1477)	1:75:A:VAL:HG22	1:77:A:GLU:HA	8	0.13
(1,1477)	1:75:A:VAL:HG23	1:77:A:GLU:HA	8	0.13
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD11	6	0.13
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD12	6	0.13
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD13	6	0.13
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD11	6	0.13
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD12	6	0.13
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD13	6	0.13
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD11	9	0.13
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD12	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1451)	1:62:A:ASN:HB2	1:81:A:ILE:HD13	9	0.13
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD11	9	0.13
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD12	9	0.13
(1,1451)	1:62:A:ASN:HB3	1:81:A:ILE:HD13	9	0.13
(1,1440)	1:61:A:VAL:HG11	1:80:A:PHE:HZ	1	0.13
(1,1440)	1:61:A:VAL:HG12	1:80:A:PHE:HZ	1	0.13
(1,1440)	1:61:A:VAL:HG13	1:80:A:PHE:HZ	1	0.13
(1,1440)	1:61:A:VAL:HG21	1:80:A:PHE:HZ	1	0.13
(1,1440)	1:61:A:VAL:HG22	1:80:A:PHE:HZ	1	0.13
(1,1440)	1:61:A:VAL:HG23	1:80:A:PHE:HZ	1	0.13
(1,1440)	1:61:A:VAL:HG11	1:80:A:PHE:HZ	9	0.13
(1,1440)	1:61:A:VAL:HG12	1:80:A:PHE:HZ	9	0.13
(1,1440)	1:61:A:VAL:HG13	1:80:A:PHE:HZ	9	0.13
(1,1440)	1:61:A:VAL:HG21	1:80:A:PHE:HZ	9	0.13
(1,1440)	1:61:A:VAL:HG22	1:80:A:PHE:HZ	9	0.13
(1,1440)	1:61:A:VAL:HG23	1:80:A:PHE:HZ	9	0.13
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB2	6	0.13
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB3	6	0.13
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG11	8	0.13
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG12	8	0.13
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG13	8	0.13
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG21	8	0.13
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG22	8	0.13
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG23	8	0.13
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG11	8	0.13
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG12	8	0.13
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG13	8	0.13
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG21	8	0.13
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG22	8	0.13
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG23	8	0.13
(1,1357)	1:36:A:ILE:HB	1:40:A:ARG:HD2	8	0.13
(1,1357)	1:36:A:ILE:HB	1:40:A:ARG:HD3	8	0.13
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD11	3	0.13
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD12	3	0.13
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD13	3	0.13
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD21	3	0.13
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD22	3	0.13
(1,1346)	1:34:A:THR:HG21	1:106:A:LEU:HD23	3	0.13
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD11	3	0.13
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD12	3	0.13
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD13	3	0.13
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD21	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD22	3	0.13
(1,1346)	1:34:A:THR:HG22	1:106:A:LEU:HD23	3	0.13
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD11	3	0.13
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD12	3	0.13
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD13	3	0.13
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD21	3	0.13
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD22	3	0.13
(1,1346)	1:34:A:THR:HG23	1:106:A:LEU:HD23	3	0.13
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	3	0.13
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	3	0.13
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	3	0.13
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	3	0.13
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	3	0.13
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	3	0.13
(1,1316)	1:29:A:GLY:HA2	1:31:A:LYS:HD2	5	0.13
(1,1316)	1:29:A:GLY:HA2	1:31:A:LYS:HD3	5	0.13
(1,1316)	1:29:A:GLY:HA3	1:31:A:LYS:HD2	5	0.13
(1,1316)	1:29:A:GLY:HA3	1:31:A:LYS:HD3	5	0.13
(1,1316)	1:29:A:GLY:HA2	1:31:A:LYS:HD2	9	0.13
(1,1316)	1:29:A:GLY:HA2	1:31:A:LYS:HD3	9	0.13
(1,1316)	1:29:A:GLY:HA3	1:31:A:LYS:HD2	9	0.13
(1,1316)	1:29:A:GLY:HA3	1:31:A:LYS:HD3	9	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE1	6	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE2	6	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE3	6	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE1	7	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE2	7	0.13
(1,1265)	1:115:A:PHE:H	1:118:A:MET:HE3	7	0.13
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB2	8	0.13
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB3	8	0.13
(1,1196)	1:85:A:LYS:HA	1:89:A:THR:H	2	0.13
(1,1187)	1:116:A:SER:HA	1:152:A:THR:H	7	0.13
(1,1018)	1:116:A:SER:HB2	1:118:A:MET:H	10	0.13
(1,1018)	1:116:A:SER:HB3	1:118:A:MET:H	10	0.13
(1,855)	1:106:A:LEU:H	1:107:A:LYS:H	3	0.13
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE1	4	0.13
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE2	4	0.13
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE1	4	0.13
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE2	4	0.13
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE1	9	0.13
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE2	9	0.13
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE1	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE2	9	0.13
(1,753)	1:175:A:TYR:HD1	1:180:A:LYS:H	7	0.13
(1,753)	1:175:A:TYR:HD2	1:180:A:LYS:H	7	0.13
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	8	0.13
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	8	0.13
(1,739)	1:119:A:TYR:HE1	1:142:A:THR:HA	3	0.13
(1,739)	1:119:A:TYR:HE2	1:142:A:THR:HA	3	0.13
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD11	3	0.13
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD12	3	0.13
(1,708)	1:152:A:THR:H	1:156:A:ILE:HD13	3	0.13
(1,700)	1:103:A:ALA:HB1	1:115:A:PHE:HD1	8	0.13
(1,700)	1:103:A:ALA:HB1	1:115:A:PHE:HD2	8	0.13
(1,700)	1:103:A:ALA:HB2	1:115:A:PHE:HD1	8	0.13
(1,700)	1:103:A:ALA:HB2	1:115:A:PHE:HD2	8	0.13
(1,700)	1:103:A:ALA:HB3	1:115:A:PHE:HD1	8	0.13
(1,700)	1:103:A:ALA:HB3	1:115:A:PHE:HD2	8	0.13
(1,697)	1:115:A:PHE:HD1	1:156:A:ILE:HG21	9	0.13
(1,697)	1:115:A:PHE:HD1	1:156:A:ILE:HG22	9	0.13
(1,697)	1:115:A:PHE:HD1	1:156:A:ILE:HG23	9	0.13
(1,697)	1:115:A:PHE:HD2	1:156:A:ILE:HG21	9	0.13
(1,697)	1:115:A:PHE:HD2	1:156:A:ILE:HG22	9	0.13
(1,697)	1:115:A:PHE:HD2	1:156:A:ILE:HG23	9	0.13
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE1	4	0.13
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE2	4	0.13
(1,696)	1:115:A:PHE:HD1	1:118:A:MET:HE3	4	0.13
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE1	4	0.13
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE2	4	0.13
(1,696)	1:115:A:PHE:HD2	1:118:A:MET:HE3	4	0.13
(1,687)	1:55:A:ASP:HA	1:80:A:PHE:HZ	1	0.13
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD11	3	0.13
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD12	3	0.13
(1,595)	1:56:A:ALA:HB1	1:132:A:LEU:HD13	3	0.13
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD11	3	0.13
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD12	3	0.13
(1,595)	1:56:A:ALA:HB2	1:132:A:LEU:HD13	3	0.13
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD11	3	0.13
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD12	3	0.13
(1,595)	1:56:A:ALA:HB3	1:132:A:LEU:HD13	3	0.13
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD11	2	0.13
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD12	2	0.13
(1,573)	1:81:A:ILE:HG21	1:82:A:LEU:HD13	2	0.13
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD11	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD12	2	0.13
(1,573)	1:81:A:ILE:HG22	1:82:A:LEU:HD13	2	0.13
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD11	2	0.13
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD12	2	0.13
(1,573)	1:81:A:ILE:HG23	1:82:A:LEU:HD13	2	0.13
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB1	2	0.13
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB2	2	0.13
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB3	2	0.13
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB1	2	0.13
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB2	2	0.13
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB3	2	0.13
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB1	2	0.13
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB2	2	0.13
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB3	2	0.13
(1,552)	1:49:A:ILE:HG21	1:132:A:LEU:HG	6	0.13
(1,552)	1:49:A:ILE:HG22	1:132:A:LEU:HG	6	0.13
(1,552)	1:49:A:ILE:HG23	1:132:A:LEU:HG	6	0.13
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD11	7	0.13
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD12	7	0.13
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD13	7	0.13
(1,542)	1:36:A:ILE:HD11	1:40:A:ARG:HB3	5	0.13
(1,542)	1:36:A:ILE:HD12	1:40:A:ARG:HB3	5	0.13
(1,542)	1:36:A:ILE:HD13	1:40:A:ARG:HB3	5	0.13
(1,534)	1:83:A:GLU:HG3	1:178:A:LEU:HD11	1	0.13
(1,534)	1:83:A:GLU:HG3	1:178:A:LEU:HD12	1	0.13
(1,534)	1:83:A:GLU:HG3	1:178:A:LEU:HD13	1	0.13
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD21	7	0.13
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD22	7	0.13
(1,531)	1:83:A:GLU:HG2	1:178:A:LEU:HD23	7	0.13
(1,521)	1:65:A:ALA:HA	1:75:A:VAL:HG11	5	0.13
(1,521)	1:65:A:ALA:HA	1:75:A:VAL:HG12	5	0.13
(1,521)	1:65:A:ALA:HA	1:75:A:VAL:HG13	5	0.13
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	6	0.13
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	6	0.13
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	6	0.13
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	10	0.13
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	10	0.13
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	10	0.13
(1,510)	1:135:A:LEU:HD11	1:173:A:LYS:HA	5	0.13
(1,510)	1:135:A:LEU:HD12	1:173:A:LYS:HA	5	0.13
(1,510)	1:135:A:LEU:HD13	1:173:A:LYS:HA	5	0.13
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	1	0.13
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	1	0.13
(1,509)	1:45:A:ILE:HD11	1:94:A:LYS:HA	7	0.13
(1,509)	1:45:A:ILE:HD12	1:94:A:LYS:HA	7	0.13
(1,509)	1:45:A:ILE:HD13	1:94:A:LYS:HA	7	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	3	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	3	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	3	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	3	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	3	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	3	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	3	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	3	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	3	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	4	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	4	0.13
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	4	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	4	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	4	0.13
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	4	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	4	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	4	0.13
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	4	0.13
(1,403)	1:89:A:THR:HG21	1:92:A:ALA:HB1	9	0.13
(1,403)	1:89:A:THR:HG21	1:92:A:ALA:HB2	9	0.13
(1,403)	1:89:A:THR:HG21	1:92:A:ALA:HB3	9	0.13
(1,403)	1:89:A:THR:HG22	1:92:A:ALA:HB1	9	0.13
(1,403)	1:89:A:THR:HG22	1:92:A:ALA:HB2	9	0.13
(1,403)	1:89:A:THR:HG22	1:92:A:ALA:HB3	9	0.13
(1,403)	1:89:A:THR:HG23	1:92:A:ALA:HB1	9	0.13
(1,403)	1:89:A:THR:HG23	1:92:A:ALA:HB2	9	0.13
(1,403)	1:89:A:THR:HG23	1:92:A:ALA:HB3	9	0.13
(1,285)	1:83:A:GLU:HG2	1:178:A:LEU:HD11	10	0.13
(1,285)	1:83:A:GLU:HG2	1:178:A:LEU:HD12	10	0.13
(1,285)	1:83:A:GLU:HG2	1:178:A:LEU:HD13	10	0.13
(1,189)	1:49:A:ILE:HA	1:132:A:LEU:HG	1	0.13
(1,176)	1:138:A:THR:HA	1:141:A:VAL:HA	5	0.13
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE1	5	0.13
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE2	5	0.13
(1,143)	1:114:A:GLU:HA	1:118:A:MET:HE3	5	0.13
(1,98)	1:33:A:GLU:HA	1:36:A:ILE:HB	3	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD11	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD12	5	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD13	5	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD11	9	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD12	9	0.13
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD13	9	0.13
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE2	5	0.13
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE3	5	0.13
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE2	2	0.13
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE3	2	0.13
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE2	3	0.13
(1,32)	1:104:A:THR:HA	1:108:A:LYS:HE3	3	0.13
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE2	5	0.13
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE3	5	0.13
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG2	1	0.12
(1,1691)	1:128:A:PRO:HB2	1:131:A:GLU:HG3	1	0.12
(1,1670)	1:123:A:LEU:HD11	1:141:A:VAL:HB	6	0.12
(1,1670)	1:123:A:LEU:HD12	1:141:A:VAL:HB	6	0.12
(1,1670)	1:123:A:LEU:HD13	1:141:A:VAL:HB	6	0.12
(1,1670)	1:123:A:LEU:HD21	1:141:A:VAL:HB	6	0.12
(1,1670)	1:123:A:LEU:HD22	1:141:A:VAL:HB	6	0.12
(1,1670)	1:123:A:LEU:HD23	1:141:A:VAL:HB	6	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	1	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	1	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	1	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	1	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	1	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	1	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	3	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	3	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	3	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	3	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	3	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	3	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	7	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	7	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	7	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	7	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	7	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	7	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE1	10	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE2	10	0.12
(1,1616)	1:100:A:GLU:HG2	1:163:A:MET:HE3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE1	10	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE2	10	0.12
(1,1616)	1:100:A:GLU:HG3	1:163:A:MET:HE3	10	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD11	9	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD12	9	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD13	9	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD21	9	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD22	9	0.12
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD23	9	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD11	9	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD12	9	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD13	9	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD21	9	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD22	9	0.12
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD23	9	0.12
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	8	0.12
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	8	0.12
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	8	0.12
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	8	0.12
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	8	0.12
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	8	0.12
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG11	7	0.12
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG12	7	0.12
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG13	7	0.12
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG21	7	0.12
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG22	7	0.12
(1,1554)	1:89:A:THR:HG21	1:134:A:VAL:HG23	7	0.12
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG11	7	0.12
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG12	7	0.12
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG13	7	0.12
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG21	7	0.12
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG22	7	0.12
(1,1554)	1:89:A:THR:HG22	1:134:A:VAL:HG23	7	0.12
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG11	7	0.12
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG12	7	0.12
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG13	7	0.12
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG21	7	0.12
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG22	7	0.12
(1,1554)	1:89:A:THR:HG23	1:134:A:VAL:HG23	7	0.12
(1,1506)	1:82:A:LEU:HD11	1:174:A:ASN:HA	10	0.12
(1,1506)	1:82:A:LEU:HD12	1:174:A:ASN:HA	10	0.12
(1,1506)	1:82:A:LEU:HD13	1:174:A:ASN:HA	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:82:A:LEU:HD21	1:174:A:ASN:HA	10	0.12
(1,1506)	1:82:A:LEU:HD22	1:174:A:ASN:HA	10	0.12
(1,1506)	1:82:A:LEU:HD23	1:174:A:ASN:HA	10	0.12
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD11	9	0.12
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD12	9	0.12
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD13	9	0.12
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD21	9	0.12
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD22	9	0.12
(1,1499)	1:81:A:ILE:HD11	1:82:A:LEU:HD23	9	0.12
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD11	9	0.12
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD12	9	0.12
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD13	9	0.12
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD21	9	0.12
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD22	9	0.12
(1,1499)	1:81:A:ILE:HD12	1:82:A:LEU:HD23	9	0.12
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD11	9	0.12
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD12	9	0.12
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD13	9	0.12
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD21	9	0.12
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD22	9	0.12
(1,1499)	1:81:A:ILE:HD13	1:82:A:LEU:HD23	9	0.12
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD11	8	0.12
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD12	8	0.12
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD13	8	0.12
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD21	8	0.12
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD22	8	0.12
(1,1488)	1:78:A:ASN:HB2	1:82:A:LEU:HD23	8	0.12
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD11	8	0.12
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD12	8	0.12
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD13	8	0.12
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD21	8	0.12
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD22	8	0.12
(1,1488)	1:78:A:ASN:HB3	1:82:A:LEU:HD23	8	0.12
(1,1440)	1:61:A:VAL:HG11	1:80:A:PHE:HZ	2	0.12
(1,1440)	1:61:A:VAL:HG12	1:80:A:PHE:HZ	2	0.12
(1,1440)	1:61:A:VAL:HG13	1:80:A:PHE:HZ	2	0.12
(1,1440)	1:61:A:VAL:HG21	1:80:A:PHE:HZ	2	0.12
(1,1440)	1:61:A:VAL:HG22	1:80:A:PHE:HZ	2	0.12
(1,1440)	1:61:A:VAL:HG23	1:80:A:PHE:HZ	2	0.12
(1,1420)	1:56:A:ALA:HB1	1:61:A:VAL:HG11	2	0.12
(1,1420)	1:56:A:ALA:HB1	1:61:A:VAL:HG12	2	0.12
(1,1420)	1:56:A:ALA:HB1	1:61:A:VAL:HG13	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:56:A:ALA:HB1	1:61:A:VAL:HG21	2	0.12
(1,1420)	1:56:A:ALA:HB1	1:61:A:VAL:HG22	2	0.12
(1,1420)	1:56:A:ALA:HB1	1:61:A:VAL:HG23	2	0.12
(1,1420)	1:56:A:ALA:HB2	1:61:A:VAL:HG11	2	0.12
(1,1420)	1:56:A:ALA:HB2	1:61:A:VAL:HG12	2	0.12
(1,1420)	1:56:A:ALA:HB2	1:61:A:VAL:HG13	2	0.12
(1,1420)	1:56:A:ALA:HB2	1:61:A:VAL:HG21	2	0.12
(1,1420)	1:56:A:ALA:HB2	1:61:A:VAL:HG22	2	0.12
(1,1420)	1:56:A:ALA:HB2	1:61:A:VAL:HG23	2	0.12
(1,1420)	1:56:A:ALA:HB3	1:61:A:VAL:HG11	2	0.12
(1,1420)	1:56:A:ALA:HB3	1:61:A:VAL:HG12	2	0.12
(1,1420)	1:56:A:ALA:HB3	1:61:A:VAL:HG13	2	0.12
(1,1420)	1:56:A:ALA:HB3	1:61:A:VAL:HG21	2	0.12
(1,1420)	1:56:A:ALA:HB3	1:61:A:VAL:HG22	2	0.12
(1,1420)	1:56:A:ALA:HB3	1:61:A:VAL:HG23	2	0.12
(1,1361)	1:36:A:ILE:HG12	1:40:A:ARG:HD2	5	0.12
(1,1361)	1:36:A:ILE:HG12	1:40:A:ARG:HD3	5	0.12
(1,1361)	1:36:A:ILE:HG13	1:40:A:ARG:HD2	5	0.12
(1,1361)	1:36:A:ILE:HG13	1:40:A:ARG:HD3	5	0.12
(1,1357)	1:36:A:ILE:HB	1:40:A:ARG:HD2	7	0.12
(1,1357)	1:36:A:ILE:HB	1:40:A:ARG:HD3	7	0.12
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	7	0.12
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	7	0.12
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	7	0.12
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	7	0.12
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	7	0.12
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	7	0.12
(1,1331)	1:30:A:LEU:HD11	1:34:A:THR:H	3	0.12
(1,1331)	1:30:A:LEU:HD12	1:34:A:THR:H	3	0.12
(1,1331)	1:30:A:LEU:HD13	1:34:A:THR:H	3	0.12
(1,1331)	1:30:A:LEU:HD21	1:34:A:THR:H	3	0.12
(1,1331)	1:30:A:LEU:HD22	1:34:A:THR:H	3	0.12
(1,1331)	1:30:A:LEU:HD23	1:34:A:THR:H	3	0.12
(1,1331)	1:30:A:LEU:HD11	1:34:A:THR:H	5	0.12
(1,1331)	1:30:A:LEU:HD12	1:34:A:THR:H	5	0.12
(1,1331)	1:30:A:LEU:HD13	1:34:A:THR:H	5	0.12
(1,1331)	1:30:A:LEU:HD21	1:34:A:THR:H	5	0.12
(1,1331)	1:30:A:LEU:HD22	1:34:A:THR:H	5	0.12
(1,1331)	1:30:A:LEU:HD23	1:34:A:THR:H	5	0.12
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE2	4	0.12
(1,1330)	1:30:A:LEU:HD11	1:31:A:LYS:HE3	4	0.12
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:30:A:LEU:HD12	1:31:A:LYS:HE3	4	0.12
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE2	4	0.12
(1,1330)	1:30:A:LEU:HD13	1:31:A:LYS:HE3	4	0.12
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE2	4	0.12
(1,1330)	1:30:A:LEU:HD21	1:31:A:LYS:HE3	4	0.12
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE2	4	0.12
(1,1330)	1:30:A:LEU:HD22	1:31:A:LYS:HE3	4	0.12
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE2	4	0.12
(1,1330)	1:30:A:LEU:HD23	1:31:A:LYS:HE3	4	0.12
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	4	0.12
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	4	0.12
(1,1143)	1:180:A:LYS:HB2	1:182:A:LYS:H	7	0.12
(1,1143)	1:180:A:LYS:HB3	1:182:A:LYS:H	7	0.12
(1,1137)	1:172:A:THR:HG21	1:174:A:ASN:H	3	0.12
(1,1137)	1:172:A:THR:HG22	1:174:A:ASN:H	3	0.12
(1,1137)	1:172:A:THR:HG23	1:174:A:ASN:H	3	0.12
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG12	1	0.12
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG13	1	0.12
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG12	7	0.12
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG13	7	0.12
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE1	4	0.12
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE2	4	0.12
(1,756)	1:175:A:TYR:HD1	1:178:A:LEU:HG	7	0.12
(1,756)	1:175:A:TYR:HD2	1:178:A:LEU:HG	7	0.12
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	6	0.12
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	6	0.12
(1,748)	1:119:A:TYR:HE1	1:123:A:LEU:HB3	10	0.12
(1,748)	1:119:A:TYR:HE2	1:123:A:LEU:HB3	10	0.12
(1,743)	1:119:A:TYR:HE1	1:123:A:LEU:HA	8	0.12
(1,743)	1:119:A:TYR:HE2	1:123:A:LEU:HA	8	0.12
(1,739)	1:119:A:TYR:HE1	1:142:A:THR:HA	4	0.12
(1,739)	1:119:A:TYR:HE2	1:142:A:THR:HA	4	0.12
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	10	0.12
(1,718)	1:67:A:THR:HG21	1:68:A:ASP:HA	7	0.12
(1,718)	1:67:A:THR:HG22	1:68:A:ASP:HA	7	0.12
(1,718)	1:67:A:THR:HG23	1:68:A:ASP:HA	7	0.12
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	3	0.12
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	3	0.12
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	4	0.12
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	4	0.12
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	6	0.12
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE1	10	0.12
(1,681)	1:63:A:PHE:HA	1:63:A:PHE:HE2	10	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	3	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	3	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	3	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	5	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	5	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	5	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	8	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	8	0.12
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	8	0.12
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB1	9	0.12
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB2	9	0.12
(1,565)	1:52:A:ILE:HD11	1:88:A:ALA:HB3	9	0.12
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB1	9	0.12
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB2	9	0.12
(1,565)	1:52:A:ILE:HD12	1:88:A:ALA:HB3	9	0.12
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB1	9	0.12
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB2	9	0.12
(1,565)	1:52:A:ILE:HD13	1:88:A:ALA:HB3	9	0.12
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE1	4	0.12
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE2	4	0.12
(1,559)	1:156:A:ILE:HG21	1:163:A:MET:HE3	4	0.12
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE1	4	0.12
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE2	4	0.12
(1,559)	1:156:A:ILE:HG22	1:163:A:MET:HE3	4	0.12
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE1	4	0.12
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE2	4	0.12
(1,559)	1:156:A:ILE:HG23	1:163:A:MET:HE3	4	0.12
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD11	1	0.12
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD12	1	0.12
(1,555)	1:151:A:THR:HG21	1:156:A:ILE:HD13	1	0.12
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD11	1	0.12
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD12	1	0.12
(1,555)	1:151:A:THR:HG22	1:156:A:ILE:HD13	1	0.12
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD11	1	0.12
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD12	1	0.12
(1,555)	1:151:A:THR:HG23	1:156:A:ILE:HD13	1	0.12
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD11	3	0.12
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD12	3	0.12
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD13	3	0.12
(1,542)	1:36:A:ILE:HD11	1:40:A:ARG:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:36:A:ILE:HD12	1:40:A:ARG:HB3	2	0.12
(1,542)	1:36:A:ILE:HD13	1:40:A:ARG:HB3	2	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	1	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	1	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	1	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	2	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	2	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	2	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	4	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	4	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	4	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	5	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	5	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	5	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	7	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	7	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	7	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	8	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	8	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	8	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	9	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	9	0.12
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	9	0.12
(1,508)	1:36:A:ILE:HG21	1:40:A:ARG:HA	5	0.12
(1,508)	1:36:A:ILE:HG22	1:40:A:ARG:HA	5	0.12
(1,508)	1:36:A:ILE:HG23	1:40:A:ARG:HA	5	0.12
(1,492)	1:97:A:THR:HB	1:167:A:LEU:HG	3	0.12
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG21	9	0.12
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG22	9	0.12
(1,444)	1:65:A:ALA:HA	1:67:A:THR:HG23	9	0.12
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	1	0.12
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	1	0.12
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	1	0.12
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	1	0.12
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	1	0.12
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	1	0.12
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	1	0.12
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	1	0.12
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	1	0.12
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	7	0.12
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	7	0.12
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	7	0.12
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	7	0.12
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	7	0.12
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	7	0.12
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	7	0.12
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	7	0.12
(1,400)	1:92:A:ALA:HB1	1:129:A:LEU:HG	7	0.12
(1,400)	1:92:A:ALA:HB2	1:129:A:LEU:HG	7	0.12
(1,400)	1:92:A:ALA:HB3	1:129:A:LEU:HG	7	0.12
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB1	1	0.12
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB2	1	0.12
(1,354)	1:82:A:LEU:HG	1:177:A:ALA:HB3	1	0.12
(1,329)	1:96:A:VAL:HB	1:167:A:LEU:HG	1	0.12
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE1	6	0.12
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE2	6	0.12
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE3	6	0.12
(1,286)	1:53:A:LYS:HE2	1:132:A:LEU:HG	6	0.12
(1,286)	1:53:A:LYS:HE3	1:132:A:LEU:HG	6	0.12
(1,237)	1:165:A:THR:HG21	1:169:A:ARG:HD2	8	0.12
(1,237)	1:165:A:THR:HG21	1:169:A:ARG:HD3	8	0.12
(1,237)	1:165:A:THR:HG22	1:169:A:ARG:HD2	8	0.12
(1,237)	1:165:A:THR:HG22	1:169:A:ARG:HD3	8	0.12
(1,237)	1:165:A:THR:HG23	1:169:A:ARG:HD2	8	0.12
(1,237)	1:165:A:THR:HG23	1:169:A:ARG:HD3	8	0.12
(1,229)	1:83:A:GLU:HG3	1:87:A:ARG:HD3	9	0.12
(1,200)	1:137:A:MET:HE1	1:141:A:VAL:HA	3	0.12
(1,200)	1:137:A:MET:HE2	1:141:A:VAL:HA	3	0.12
(1,200)	1:137:A:MET:HE3	1:141:A:VAL:HA	3	0.12
(1,197)	1:56:A:ALA:HA	1:61:A:VAL:HG11	5	0.12
(1,197)	1:56:A:ALA:HA	1:61:A:VAL:HG12	5	0.12
(1,197)	1:56:A:ALA:HA	1:61:A:VAL:HG13	5	0.12
(1,141)	1:103:A:ALA:HA	1:118:A:MET:HE1	10	0.12
(1,141)	1:103:A:ALA:HA	1:118:A:MET:HE2	10	0.12
(1,141)	1:103:A:ALA:HA	1:118:A:MET:HE3	10	0.12
(1,121)	1:89:A:THR:HG21	1:171:A:HIS:HA	2	0.12
(1,121)	1:89:A:THR:HG22	1:171:A:HIS:HA	2	0.12
(1,121)	1:89:A:THR:HG23	1:171:A:HIS:HA	2	0.12
(1,98)	1:33:A:GLU:HA	1:36:A:ILE:HB	1	0.12
(1,98)	1:33:A:GLU:HA	1:36:A:ILE:HB	4	0.12
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD11	8	0.12
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD12	8	0.12
(1,83)	1:76:A:SER:HA	1:81:A:ILE:HD13	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:65:A:ALA:HA	1:68:A:ASP:HB2	5	0.12
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE2	1	0.12
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE3	1	0.12
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE2	7	0.12
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE3	7	0.12
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB1	4	0.12
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB2	4	0.12
(1,18)	1:174:A:ASN:HA	1:177:A:ALA:HB3	4	0.12
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE2	6	0.12
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE3	6	0.12
(1,1687)	1:125:A:VAL:HG11	1:129:A:LEU:HB3	10	0.11
(1,1687)	1:125:A:VAL:HG12	1:129:A:LEU:HB3	10	0.11
(1,1687)	1:125:A:VAL:HG13	1:129:A:LEU:HB3	10	0.11
(1,1687)	1:125:A:VAL:HG21	1:129:A:LEU:HB3	10	0.11
(1,1687)	1:125:A:VAL:HG22	1:129:A:LEU:HB3	10	0.11
(1,1687)	1:125:A:VAL:HG23	1:129:A:LEU:HB3	10	0.11
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD11	6	0.11
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD12	6	0.11
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD13	6	0.11
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD21	6	0.11
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD22	6	0.11
(1,1614)	1:100:A:GLU:HG2	1:157:A:LEU:HD23	6	0.11
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD11	6	0.11
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD12	6	0.11
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD13	6	0.11
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD21	6	0.11
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD22	6	0.11
(1,1614)	1:100:A:GLU:HG3	1:157:A:LEU:HD23	6	0.11
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE1	2	0.11
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE2	2	0.11
(1,1604)	1:99:A:ILE:HG12	1:118:A:MET:HE3	2	0.11
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE1	2	0.11
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE2	2	0.11
(1,1604)	1:99:A:ILE:HG13	1:118:A:MET:HE3	2	0.11
(1,1591)	1:96:A:VAL:HG11	1:167:A:LEU:HG	3	0.11
(1,1591)	1:96:A:VAL:HG12	1:167:A:LEU:HG	3	0.11
(1,1591)	1:96:A:VAL:HG13	1:167:A:LEU:HG	3	0.11
(1,1591)	1:96:A:VAL:HG21	1:167:A:LEU:HG	3	0.11
(1,1591)	1:96:A:VAL:HG22	1:167:A:LEU:HG	3	0.11
(1,1591)	1:96:A:VAL:HG23	1:167:A:LEU:HG	3	0.11
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD2	10	0.11
(1,1526)	1:84:A:ALA:HB1	1:87:A:ARG:HD3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD2	10	0.11
(1,1526)	1:84:A:ALA:HB2	1:87:A:ARG:HD3	10	0.11
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD2	10	0.11
(1,1526)	1:84:A:ALA:HB3	1:87:A:ARG:HD3	10	0.11
(1,1506)	1:82:A:LEU:HD11	1:174:A:ASN:HA	8	0.11
(1,1506)	1:82:A:LEU:HD12	1:174:A:ASN:HA	8	0.11
(1,1506)	1:82:A:LEU:HD13	1:174:A:ASN:HA	8	0.11
(1,1506)	1:82:A:LEU:HD21	1:174:A:ASN:HA	8	0.11
(1,1506)	1:82:A:LEU:HD22	1:174:A:ASN:HA	8	0.11
(1,1506)	1:82:A:LEU:HD23	1:174:A:ASN:HA	8	0.11
(1,1477)	1:75:A:VAL:HG11	1:77:A:GLU:HA	7	0.11
(1,1477)	1:75:A:VAL:HG12	1:77:A:GLU:HA	7	0.11
(1,1477)	1:75:A:VAL:HG13	1:77:A:GLU:HA	7	0.11
(1,1477)	1:75:A:VAL:HG21	1:77:A:GLU:HA	7	0.11
(1,1477)	1:75:A:VAL:HG22	1:77:A:GLU:HA	7	0.11
(1,1477)	1:75:A:VAL:HG23	1:77:A:GLU:HA	7	0.11
(1,1474)	1:70:A:GLU:HG2	1:71:A:THR:HA	8	0.11
(1,1474)	1:70:A:GLU:HG3	1:71:A:THR:HA	8	0.11
(1,1456)	1:65:A:ALA:H	1:76:A:SER:HB2	1	0.11
(1,1456)	1:65:A:ALA:H	1:76:A:SER:HB3	1	0.11
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB2	7	0.11
(1,1424)	1:59:A:ASN:H	1:60:A:ASN:HB3	7	0.11
(1,1394)	1:45:A:ILE:HG12	1:95:A:PHE:HA	8	0.11
(1,1394)	1:45:A:ILE:HG13	1:95:A:PHE:HA	8	0.11
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	8	0.11
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	8	0.11
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	8	0.11
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	8	0.11
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	8	0.11
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	8	0.11
(1,1324)	1:30:A:LEU:HB2	1:35:A:LYS:H	9	0.11
(1,1324)	1:30:A:LEU:HB3	1:35:A:LYS:H	9	0.11
(1,1300)	1:150:A:THR:HG21	1:152:A:THR:H	2	0.11
(1,1300)	1:150:A:THR:HG22	1:152:A:THR:H	2	0.11
(1,1300)	1:150:A:THR:HG23	1:152:A:THR:H	2	0.11
(1,1300)	1:150:A:THR:HG21	1:152:A:THR:H	8	0.11
(1,1300)	1:150:A:THR:HG22	1:152:A:THR:H	8	0.11
(1,1300)	1:150:A:THR:HG23	1:152:A:THR:H	8	0.11
(1,1224)	1:164:A:LYS:HB2	1:166:A:LYS:H	1	0.11
(1,1224)	1:164:A:LYS:HB3	1:166:A:LYS:H	1	0.11
(1,1224)	1:164:A:LYS:HB2	1:166:A:LYS:H	2	0.11
(1,1224)	1:164:A:LYS:HB3	1:166:A:LYS:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:164:A:LYS:HB2	1:166:A:LYS:H	10	0.11
(1,1224)	1:164:A:LYS:HB3	1:166:A:LYS:H	10	0.11
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB2	4	0.11
(1,1221)	1:105:A:LYS:H	1:107:A:LYS:HB3	4	0.11
(1,1179)	1:101:A:GLY:HA3	1:104:A:THR:H	8	0.11
(1,1162)	1:109:A:THR:HB	1:116:A:SER:H	10	0.11
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	8	0.11
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG12	6	0.11
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG13	6	0.11
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG12	8	0.11
(1,1065)	1:49:A:ILE:H	1:52:A:ILE:HG13	8	0.11
(1,898)	1:52:A:ILE:HD11	1:87:A:ARG:H	8	0.11
(1,898)	1:52:A:ILE:HD12	1:87:A:ARG:H	8	0.11
(1,898)	1:52:A:ILE:HD13	1:87:A:ARG:H	8	0.11
(1,879)	1:75:A:VAL:HB	1:77:A:GLU:H	5	0.11
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	3	0.11
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	3	0.11
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	3	0.11
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE1	8	0.11
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE2	8	0.11
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE1	10	0.11
(1,809)	1:52:A:ILE:HA	1:63:A:PHE:HE2	10	0.11
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE1	6	0.11
(1,801)	1:53:A:LYS:HE2	1:66:A:PHE:HE2	6	0.11
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE1	6	0.11
(1,801)	1:53:A:LYS:HE3	1:66:A:PHE:HE2	6	0.11
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE1	1	0.11
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE2	1	0.11
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE1	7	0.11
(1,794)	1:179:A:GLU:HA	1:186:A:PHE:HE2	7	0.11
(1,778)	1:66:A:PHE:HD1	1:132:A:LEU:HB2	1	0.11
(1,778)	1:66:A:PHE:HD2	1:132:A:LEU:HB2	1	0.11
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE1	10	0.11
(1,740)	1:175:A:TYR:HA	1:175:A:TYR:HE2	10	0.11
(1,739)	1:119:A:TYR:HE1	1:142:A:THR:HA	6	0.11
(1,739)	1:119:A:TYR:HE2	1:142:A:THR:HA	6	0.11
(1,739)	1:119:A:TYR:HE1	1:142:A:THR:HA	7	0.11
(1,739)	1:119:A:TYR:HE2	1:142:A:THR:HA	7	0.11
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	1	0.11
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	2	0.11
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG21	3	0.11
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG22	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:42:A:ALA:HA	1:45:A:ILE:HG23	3	0.11
(1,721)	1:61:A:VAL:HG21	1:63:A:PHE:HA	7	0.11
(1,721)	1:61:A:VAL:HG22	1:63:A:PHE:HA	7	0.11
(1,721)	1:61:A:VAL:HG23	1:63:A:PHE:HA	7	0.11
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD1	3	0.11
(1,688)	1:103:A:ALA:HA	1:115:A:PHE:HD2	3	0.11
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	7	0.11
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	7	0.11
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	7	0.11
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG21	7	0.11
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG22	7	0.11
(1,556)	1:151:A:THR:HG21	1:156:A:ILE:HG23	7	0.11
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG21	7	0.11
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG22	7	0.11
(1,556)	1:151:A:THR:HG22	1:156:A:ILE:HG23	7	0.11
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG21	7	0.11
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG22	7	0.11
(1,556)	1:151:A:THR:HG23	1:156:A:ILE:HG23	7	0.11
(1,542)	1:36:A:ILE:HD11	1:40:A:ARG:HB3	8	0.11
(1,542)	1:36:A:ILE:HD12	1:40:A:ARG:HB3	8	0.11
(1,542)	1:36:A:ILE:HD13	1:40:A:ARG:HB3	8	0.11
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG21	3	0.11
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG22	3	0.11
(1,525)	1:153:A:ALA:HA	1:156:A:ILE:HG23	3	0.11
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG21	4	0.11
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG22	4	0.11
(1,522)	1:65:A:ALA:HA	1:75:A:VAL:HG23	4	0.11
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG21	3	0.11
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG22	3	0.11
(1,513)	1:161:A:LYS:HA	1:162:A:ILE:HG23	3	0.11
(1,492)	1:97:A:THR:HB	1:167:A:LEU:HG	10	0.11
(1,462)	1:37:A:ILE:HG12	1:40:A:ARG:HB3	2	0.11
(1,462)	1:37:A:ILE:HG13	1:40:A:ARG:HB3	2	0.11
(1,447)	1:97:A:THR:HG21	1:101:A:GLY:HA2	5	0.11
(1,447)	1:97:A:THR:HG22	1:101:A:GLY:HA2	5	0.11
(1,447)	1:97:A:THR:HG23	1:101:A:GLY:HA2	5	0.11
(1,447)	1:97:A:THR:HG21	1:101:A:GLY:HA2	8	0.11
(1,447)	1:97:A:THR:HG22	1:101:A:GLY:HA2	8	0.11
(1,447)	1:97:A:THR:HG23	1:101:A:GLY:HA2	8	0.11
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG21	9	0.11
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG22	9	0.11
(1,411)	1:92:A:ALA:HB1	1:125:A:VAL:HG23	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG21	9	0.11
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG22	9	0.11
(1,411)	1:92:A:ALA:HB2	1:125:A:VAL:HG23	9	0.11
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG21	9	0.11
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG22	9	0.11
(1,411)	1:92:A:ALA:HB3	1:125:A:VAL:HG23	9	0.11
(1,398)	1:128:A:PRO:HB2	1:131:A:GLU:HG3	2	0.11
(1,391)	1:56:A:ALA:HB1	1:62:A:ASN:HA	2	0.11
(1,391)	1:56:A:ALA:HB2	1:62:A:ASN:HA	2	0.11
(1,391)	1:56:A:ALA:HB3	1:62:A:ASN:HA	2	0.11
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE1	3	0.11
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE2	3	0.11
(1,311)	1:99:A:ILE:HA	1:122:A:MET:HE3	3	0.11
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	10	0.11
(1,305)	1:149:A:PRO:HB3	1:152:A:THR:HB	7	0.11
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG21	5	0.11
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG22	5	0.11
(1,242)	1:119:A:TYR:HB2	1:150:A:THR:HG23	5	0.11
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD11	6	0.11
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD12	6	0.11
(1,219)	1:119:A:TYR:HB3	1:156:A:ILE:HD13	6	0.11
(1,200)	1:137:A:MET:HE1	1:141:A:VAL:HA	1	0.11
(1,200)	1:137:A:MET:HE2	1:141:A:VAL:HA	1	0.11
(1,200)	1:137:A:MET:HE3	1:141:A:VAL:HA	1	0.11
(1,189)	1:49:A:ILE:HA	1:132:A:LEU:HG	6	0.11
(1,172)	1:99:A:ILE:HD11	1:118:A:MET:HA	1	0.11
(1,172)	1:99:A:ILE:HD12	1:118:A:MET:HA	1	0.11
(1,172)	1:99:A:ILE:HD13	1:118:A:MET:HA	1	0.11
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	4	0.11
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	4	0.11
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	4	0.11
(1,167)	1:49:A:ILE:HD11	1:132:A:LEU:HA	5	0.11
(1,167)	1:49:A:ILE:HD12	1:132:A:LEU:HA	5	0.11
(1,167)	1:49:A:ILE:HD13	1:132:A:LEU:HA	5	0.11
(1,157)	1:45:A:ILE:HG21	1:125:A:VAL:HA	1	0.11
(1,157)	1:45:A:ILE:HG22	1:125:A:VAL:HA	1	0.11
(1,157)	1:45:A:ILE:HG23	1:125:A:VAL:HA	1	0.11
(1,156)	1:140:A:THR:HA	1:162:A:ILE:HG21	10	0.11
(1,156)	1:140:A:THR:HA	1:162:A:ILE:HG22	10	0.11
(1,156)	1:140:A:THR:HA	1:162:A:ILE:HG23	10	0.11
(1,114)	1:175:A:TYR:HA	1:178:A:LEU:HD11	1	0.11
(1,114)	1:175:A:TYR:HA	1:178:A:LEU:HD12	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:175:A:TYR:HA	1:178:A:LEU:HD13	1	0.11
(1,98)	1:33:A:GLU:HA	1:36:A:ILE:HB	2	0.11
(1,90)	1:84:A:ALA:HA	1:87:A:ARG:HD2	6	0.11
(1,90)	1:84:A:ALA:HA	1:87:A:ARG:HD2	8	0.11
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD11	7	0.11
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD12	7	0.11
(1,81)	1:144:A:ALA:HA	1:159:A:ILE:HD13	7	0.11
(1,70)	1:115:A:PHE:HA	1:156:A:ILE:HG21	10	0.11
(1,70)	1:115:A:PHE:HA	1:156:A:ILE:HG22	10	0.11
(1,70)	1:115:A:PHE:HA	1:156:A:ILE:HG23	10	0.11
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE2	2	0.11
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE3	2	0.11
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE2	3	0.11
(1,6)	1:31:A:LYS:HA	1:31:A:LYS:HE3	3	0.11
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD11	5	0.1
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD12	5	0.1
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD13	5	0.1
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD21	5	0.1
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD22	5	0.1
(1,1659)	1:120:A:ASN:HA	1:123:A:LEU:HD23	5	0.1
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE2	8	0.1
(1,1617)	1:102:A:GLU:HB2	1:108:A:LYS:HE3	8	0.1
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE2	8	0.1
(1,1617)	1:102:A:GLU:HB3	1:108:A:LYS:HE3	8	0.1
(1,1471)	1:69:A:SER:HB2	1:70:A:GLU:HG2	9	0.1
(1,1471)	1:69:A:SER:HB2	1:70:A:GLU:HG3	9	0.1
(1,1471)	1:69:A:SER:HB3	1:70:A:GLU:HG2	9	0.1
(1,1471)	1:69:A:SER:HB3	1:70:A:GLU:HG3	9	0.1
(1,1456)	1:65:A:ALA:H	1:76:A:SER:HB2	10	0.1
(1,1456)	1:65:A:ALA:H	1:76:A:SER:HB3	10	0.1
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG11	2	0.1
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG12	2	0.1
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG13	2	0.1
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG21	2	0.1
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG22	2	0.1
(1,1384)	1:44:A:ASP:HB2	1:91:A:VAL:HG23	2	0.1
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG11	2	0.1
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG12	2	0.1
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG13	2	0.1
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG21	2	0.1
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG22	2	0.1
(1,1384)	1:44:A:ASP:HB3	1:91:A:VAL:HG23	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	4	0.1
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	4	0.1
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	4	0.1
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	4	0.1
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	4	0.1
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	4	0.1
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB2	6	0.1
(1,1345)	1:34:A:THR:HG21	1:35:A:LYS:HB3	6	0.1
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB2	6	0.1
(1,1345)	1:34:A:THR:HG22	1:35:A:LYS:HB3	6	0.1
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB2	6	0.1
(1,1345)	1:34:A:THR:HG23	1:35:A:LYS:HB3	6	0.1
(1,1331)	1:30:A:LEU:HD11	1:34:A:THR:H	6	0.1
(1,1331)	1:30:A:LEU:HD12	1:34:A:THR:H	6	0.1
(1,1331)	1:30:A:LEU:HD13	1:34:A:THR:H	6	0.1
(1,1331)	1:30:A:LEU:HD21	1:34:A:THR:H	6	0.1
(1,1331)	1:30:A:LEU:HD22	1:34:A:THR:H	6	0.1
(1,1331)	1:30:A:LEU:HD23	1:34:A:THR:H	6	0.1
(1,1224)	1:164:A:LYS:HB2	1:166:A:LYS:H	9	0.1
(1,1224)	1:164:A:LYS:HB3	1:166:A:LYS:H	9	0.1
(1,1094)	1:191:A:CYS:H	1:192:A:LYS:H	1	0.1
(1,1060)	1:177:A:ALA:HB1	1:181:A:LYS:H	4	0.1
(1,1060)	1:177:A:ALA:HB2	1:181:A:LYS:H	4	0.1
(1,1060)	1:177:A:ALA:HB3	1:181:A:LYS:H	4	0.1
(1,821)	1:56:A:ALA:HB1	1:63:A:PHE:HZ	10	0.1
(1,821)	1:56:A:ALA:HB2	1:63:A:PHE:HZ	10	0.1
(1,821)	1:56:A:ALA:HB3	1:63:A:PHE:HZ	10	0.1
(1,786)	1:66:A:PHE:HD1	1:132:A:LEU:HG	1	0.1
(1,786)	1:66:A:PHE:HD2	1:132:A:LEU:HG	1	0.1
(1,747)	1:175:A:TYR:HE1	1:178:A:LEU:HG	1	0.1
(1,747)	1:175:A:TYR:HE2	1:178:A:LEU:HG	1	0.1
(1,732)	1:148:A:HIS:HB2	1:155:A:GLY:HA3	6	0.1
(1,692)	1:63:A:PHE:HB2	1:80:A:PHE:HZ	1	0.1
(1,692)	1:63:A:PHE:HB3	1:80:A:PHE:HZ	1	0.1
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG21	6	0.1
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG22	6	0.1
(1,584)	1:149:A:PRO:HA	1:150:A:THR:HG23	6	0.1
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD11	5	0.1
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD12	5	0.1
(1,548)	1:149:A:PRO:HG3	1:159:A:ILE:HD13	5	0.1
(1,485)	1:42:A:ALA:HB1	1:45:A:ILE:HD11	7	0.1
(1,485)	1:42:A:ALA:HB1	1:45:A:ILE:HD12	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,485)	1:42:A:ALA:HB1	1:45:A:ILE:HD13	7	0.1
(1,485)	1:42:A:ALA:HB2	1:45:A:ILE:HD11	7	0.1
(1,485)	1:42:A:ALA:HB2	1:45:A:ILE:HD12	7	0.1
(1,485)	1:42:A:ALA:HB2	1:45:A:ILE:HD13	7	0.1
(1,485)	1:42:A:ALA:HB3	1:45:A:ILE:HD11	7	0.1
(1,485)	1:42:A:ALA:HB3	1:45:A:ILE:HD12	7	0.1
(1,485)	1:42:A:ALA:HB3	1:45:A:ILE:HD13	7	0.1
(1,475)	1:122:A:MET:HE1	1:151:A:THR:HG21	7	0.1
(1,475)	1:122:A:MET:HE1	1:151:A:THR:HG22	7	0.1
(1,475)	1:122:A:MET:HE1	1:151:A:THR:HG23	7	0.1
(1,475)	1:122:A:MET:HE2	1:151:A:THR:HG21	7	0.1
(1,475)	1:122:A:MET:HE2	1:151:A:THR:HG22	7	0.1
(1,475)	1:122:A:MET:HE2	1:151:A:THR:HG23	7	0.1
(1,475)	1:122:A:MET:HE3	1:151:A:THR:HG21	7	0.1
(1,475)	1:122:A:MET:HE3	1:151:A:THR:HG22	7	0.1
(1,475)	1:122:A:MET:HE3	1:151:A:THR:HG23	7	0.1
(1,308)	1:164:A:LYS:HB2	1:165:A:THR:HB	9	0.1
(1,308)	1:164:A:LYS:HB3	1:165:A:THR:HB	9	0.1
(1,306)	1:140:A:THR:HB	1:162:A:ILE:HB	7	0.1
(1,179)	1:31:A:LYS:HA	1:35:A:LYS:HA	9	0.1
(1,177)	1:86:A:VAL:HA	1:171:A:HIS:HA	1	0.1
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG21	1	0.1
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG22	1	0.1
(1,132)	1:150:A:THR:HA	1:152:A:THR:HG23	1	0.1
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE2	4	0.1
(1,34)	1:94:A:LYS:HA	1:94:A:LYS:HE3	4	0.1

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

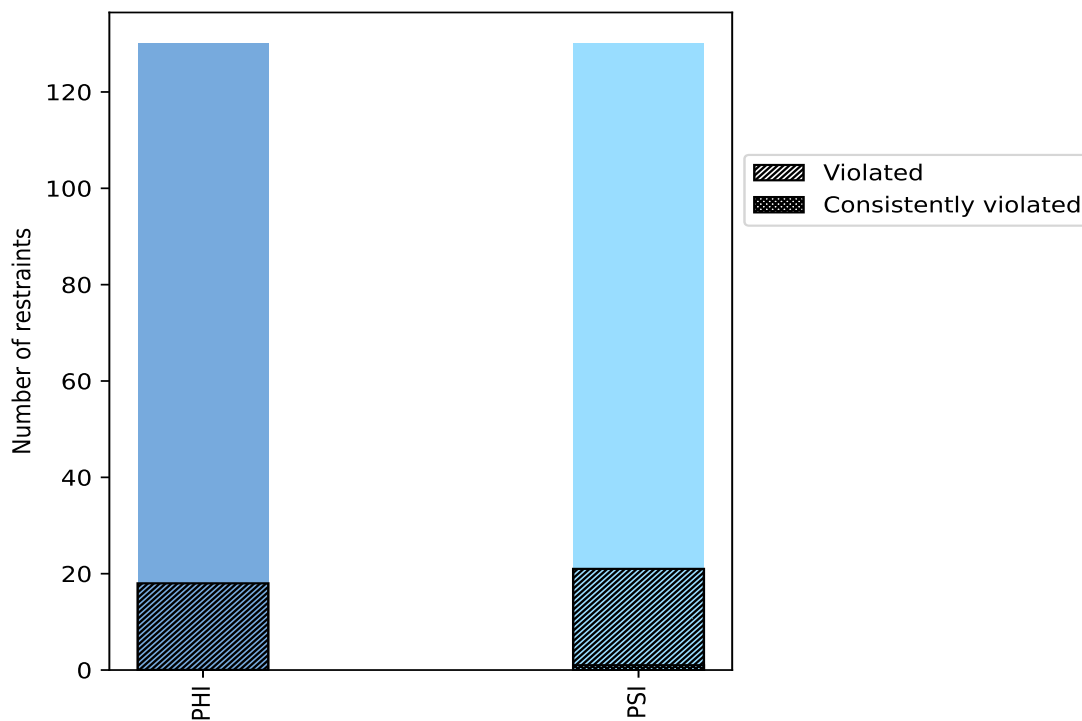
### 10.1 Summary of dihedral-angle violations [i](#)

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	130	50.0	18	13.8	6.9	0	0.0	0.0
PSI	130	50.0	21	16.2	8.1	1	0.8	0.4
Total	260	100.0	39	15.0	15.0	1	0.4	0.4

<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](#)



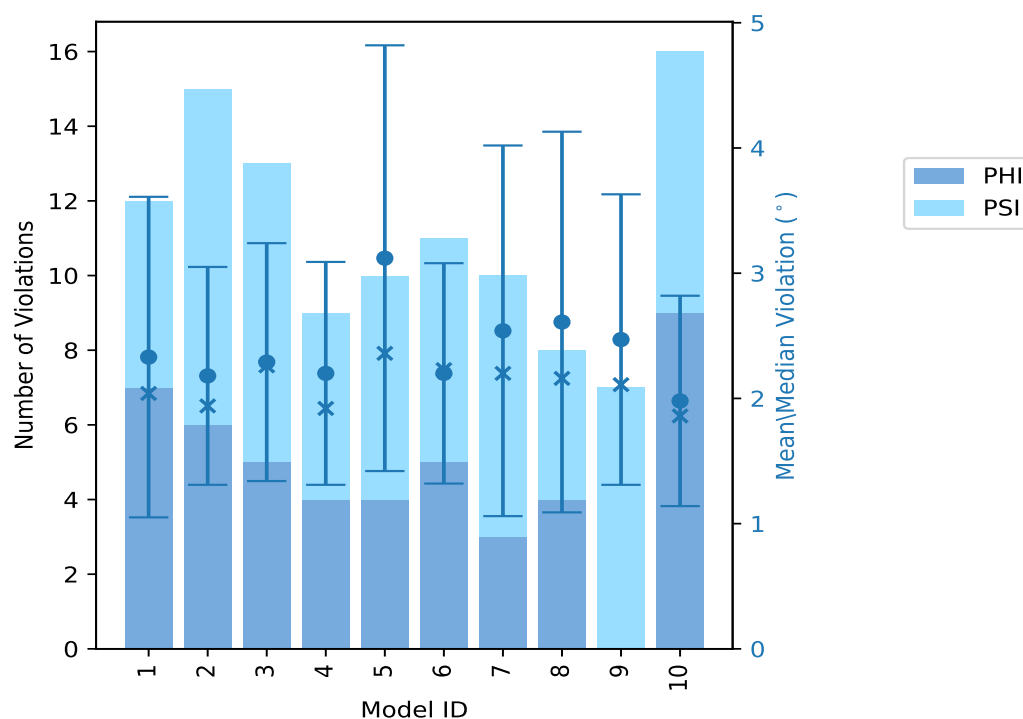
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	7	5	12	2.33	5.14	1.28	2.04
2	6	9	15	2.18	3.68	0.87	1.94
3	5	8	13	2.29	4.44	0.95	2.26
4	4	5	9	2.2	3.94	0.89	1.92
5	4	6	10	3.12	6.34	1.7	2.36
6	5	6	11	2.2	4.31	0.88	2.23
7	3	7	10	2.54	6.48	1.48	2.2
8	4	4	8	2.61	6.38	1.52	2.16
9	0	7	7	2.47	4.72	1.16	2.11
10	9	7	16	1.98	4.52	0.84	1.86

### 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

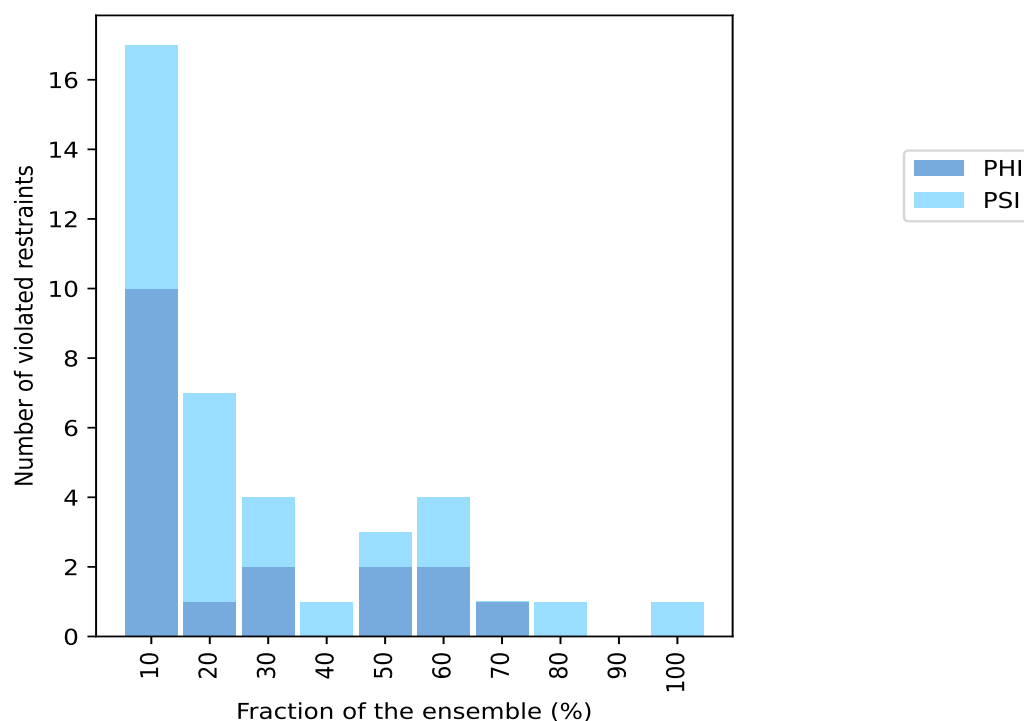
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>	%
10	7	17	1	10.0
1	6	7	2	20.0
2	2	4	3	30.0
0	1	1	4	40.0
2	1	3	5	50.0
2	2	4	6	60.0
1	0	1	7	70.0
0	1	1	8	80.0
0	0	0	9	90.0
0	1	1	10	100.0

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

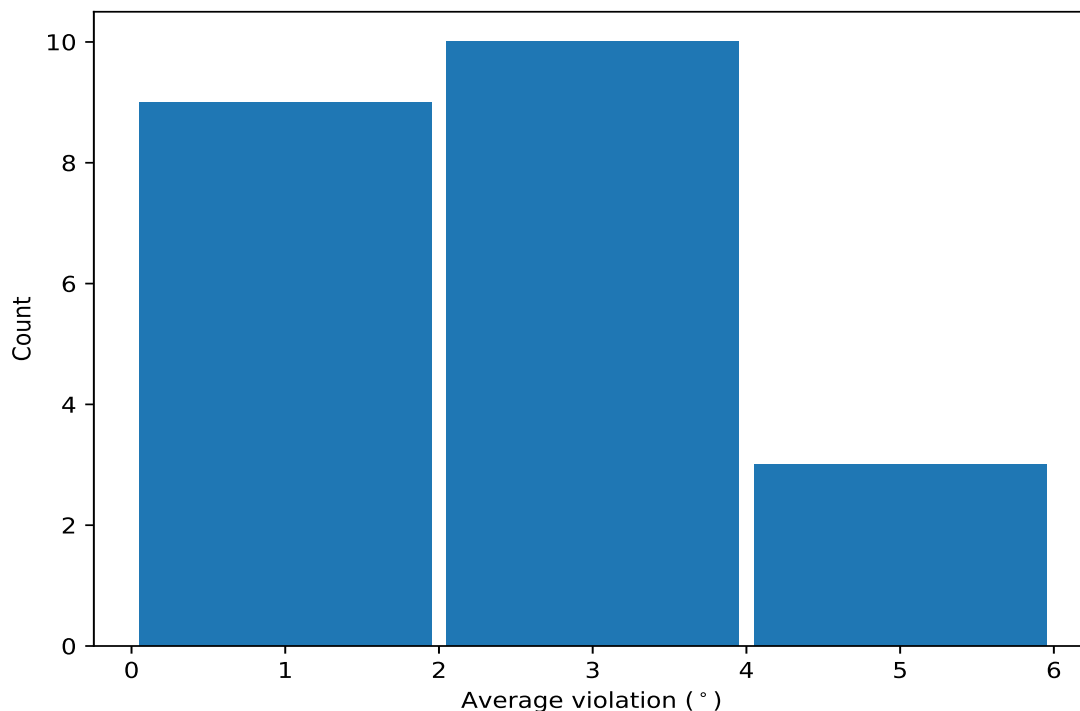
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	10	3.13	1.22	3.11
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	8	2.51	0.76	2.31
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	7	2.42	0.52	2.44
(1,132)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:GLU:N	6	2.23	0.56	2.22
(1,127)	1:108:A:LYS:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	6	2.07	1.16	1.6
(1,11)	1:36:A:ILE:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	6	1.8	0.54	1.63
(1,6)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:LYS:N	6	1.69	0.33	1.58
(1,168)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	5	4.5	1.72	5.14
(1,125)	1:107:A:LYS:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	5	4.02	1.55	4.44
(1,255)	1:190:A:LYS:C	1:191:A:CYS:N	1:191:A:CYS:CA	1:191:A:CYS:C	5	1.9	0.49	2.17
(1,200)	1:159:A:ILE:N	1:159:A:ILE:CA	1:159:A:ILE:C	1:160:A:ALA:N	4	1.35	0.24	1.27
(1,124)	1:107:A:LYS:N	1:107:A:LYS:CA	1:107:A:LYS:C	1:108:A:LYS:N	3	2.82	1.17	2.18
(1,187)	1:152:A:THR:C	1:153:A:ALA:N	1:153:A:ALA:CA	1:153:A:ALA:C	3	2.06	0.2	1.95

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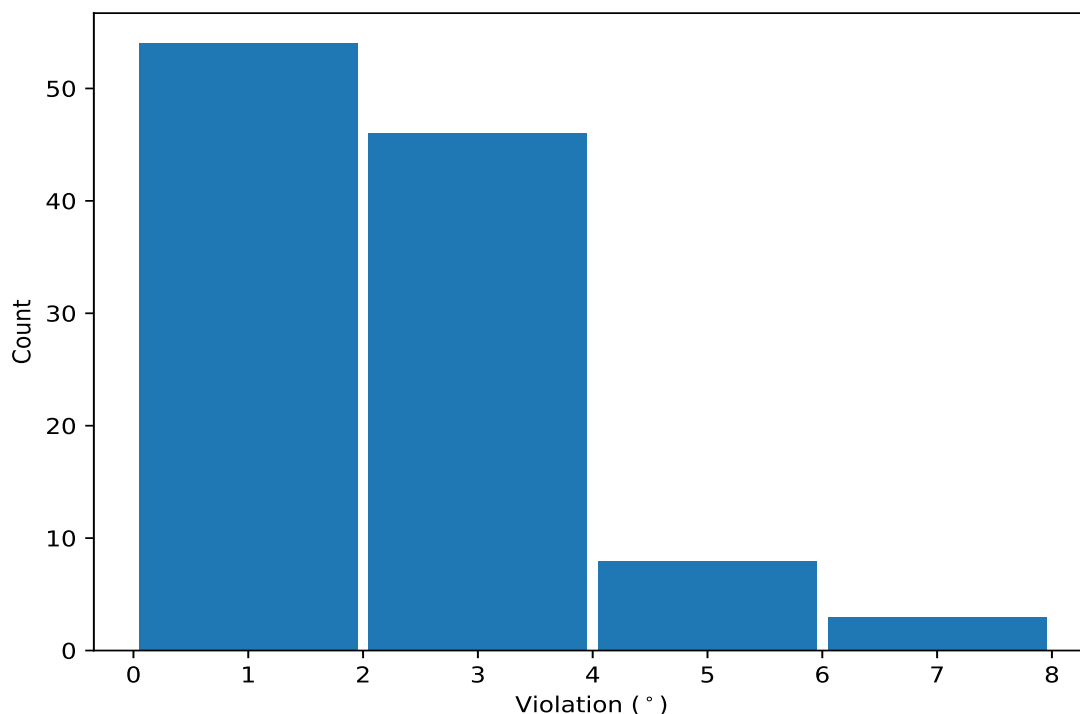
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,245)	1:184:A:PRO:C	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	3	1.55	0.37	1.41
(1,170)	1:138:A:THR:N	1:138:A:THR:CA	1:138:A:THR:C	1:139:A:LYS:N	3	1.31	0.14	1.39
(1,122)	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	1:104:A:THR:N	2	4.33	0.39	4.33
(1,246)	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	1:186:A:PHE:N	2	3.12	1.18	3.12
(1,220)	1:169:A:ARG:N	1:169:A:ARG:CA	1:169:A:ARG:C	1:170:A:VAL:N	2	2.69	0.99	2.69
(1,120)	1:102:A:GLU:N	1:102:A:GLU:CA	1:102:A:GLU:C	1:103:A:ALA:N	2	2.05	0.15	2.05
(1,140)	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	1:118:A:MET:N	2	1.8	0.12	1.8
(1,93)	1:88:A:ALA:C	1:89:A:THR:N	1:89:A:THR:CA	1:89:A:THR:C	2	1.53	0.09	1.53
(1,60)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:ASN:N	2	1.44	0.19	1.44

<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 (°)
(1,168)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	7	6.48
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	8	6.38
(1,125)	1:107:A:LYS:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	5	6.34
(1,168)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	5	5.92
(1,168)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	1	5.14
(1,122)	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	1:104:A:THR:N	9	4.72
(1,125)	1:107:A:LYS:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	1	4.6
(1,127)	1:108:A:LYS:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	10	4.52
(1,124)	1:107:A:LYS:N	1:107:A:LYS:CA	1:107:A:LYS:C	1:108:A:LYS:N	5	4.46
(1,125)	1:107:A:LYS:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	3	4.44
(1,246)	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	1:186:A:PHE:N	6	4.31
(1,122)	1:103:A:ALA:N	1:103:A:ALA:CA	1:103:A:ALA:C	1:104:A:THR:N	4	3.94
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	3	3.73
(1,220)	1:169:A:ARG:N	1:169:A:ARG:CA	1:169:A:ARG:C	1:170:A:VAL:N	2	3.68
(1,83)	1:83:A:GLU:C	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	2	3.63
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	4	3.46
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	2	3.42
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	10	3.41
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	2	3.3
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	1	3.21
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	7	3.2
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	9	3.17
(1,22)	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	1:43:A:LYS:N	7	3.17
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	9	3.02
(1,132)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:GLU:N	3	2.98
(1,125)	1:107:A:LYS:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	6	2.94
(1,168)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	3	2.85
(1,132)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:GLU:N	8	2.79
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	8	2.72
(1,137)	1:115:A:PHE:C	1:116:A:SER:N	1:116:A:SER:CA	1:116:A:SER:C	6	2.63
(1,11)	1:36:A:ILE:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	5	2.62
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	7	2.52
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	5	2.44
(1,11)	1:36:A:ILE:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	8	2.42
(1,247)	1:185:A:ASN:C	1:186:A:PHE:N	1:186:A:PHE:CA	1:186:A:PHE:C	6	2.35
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	4	2.35
(1,187)	1:152:A:THR:C	1:153:A:ALA:N	1:153:A:ALA:CA	1:153:A:ALA:C	4	2.34
(1,6)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:LYS:N	3	2.34
(1,255)	1:190:A:LYS:C	1:191:A:CYS:N	1:191:A:CYS:CA	1:191:A:CYS:C	2	2.32
(1,255)	1:190:A:LYS:C	1:191:A:CYS:N	1:191:A:CYS:CA	1:191:A:CYS:C	3	2.3
(1,132)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:GLU:N	10	2.3
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	5	2.27
(1,127)	1:108:A:LYS:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	6	2.26
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	3	2.26
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	6	2.23
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	6	2.22
(1,214)	1:166:A:LYS:N	1:166:A:LYS:CA	1:166:A:LYS:C	1:167:A:LEU:N	7	2.21
(1,135)	1:114:A:GLU:C	1:115:A:PHE:N	1:115:A:PHE:CA	1:115:A:PHE:C	2	2.21
(1,120)	1:102:A:GLU:N	1:102:A:GLU:CA	1:102:A:GLU:C	1:103:A:ALA:N	7	2.2
(1,124)	1:107:A:LYS:N	1:107:A:LYS:CA	1:107:A:LYS:C	1:108:A:LYS:N	1	2.18
(1,255)	1:190:A:LYS:C	1:191:A:CYS:N	1:191:A:CYS:CA	1:191:A:CYS:C	5	2.17
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	10	2.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	1	2.14
(1,132)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:GLU:N	2	2.13
(1,168)	1:132:A:LEU:N	1:132:A:LEU:CA	1:132:A:LEU:C	1:133:A:GLY:N	9	2.11
(1,245)	1:184:A:PRO:C	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	1	2.06
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	1	2.03
(1,187)	1:152:A:THR:C	1:153:A:ALA:N	1:153:A:ALA:CA	1:153:A:ALA:C	10	1.95
(1,246)	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	1:186:A:PHE:N	10	1.94
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	2	1.94
(1,140)	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	1:118:A:MET:N	10	1.92
(1,132)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:GLU:N	4	1.92
(1,10)	1:36:A:ILE:N	1:36:A:ILE:CA	1:36:A:ILE:C	1:37:A:ILE:N	5	1.92
(1,133)	1:113:A:GLY:C	1:114:A:GLU:N	1:114:A:GLU:CA	1:114:A:GLU:C	10	1.91
(1,187)	1:152:A:THR:C	1:153:A:ALA:N	1:153:A:ALA:CA	1:153:A:ALA:C	8	1.9
(1,120)	1:102:A:GLU:N	1:102:A:GLU:CA	1:102:A:GLU:C	1:103:A:ALA:N	1	1.9
(1,127)	1:108:A:LYS:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	8	1.86
(1,6)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:LYS:N	7	1.83
(1,124)	1:107:A:LYS:N	1:107:A:LYS:CA	1:107:A:LYS:C	1:108:A:LYS:N	3	1.81
(1,125)	1:107:A:LYS:C	1:108:A:LYS:N	1:108:A:LYS:CA	1:108:A:LYS:C	10	1.8
(1,200)	1:159:A:ILE:N	1:159:A:ILE:CA	1:159:A:ILE:C	1:160:A:ALA:N	9	1.76
(1,220)	1:169:A:ARG:N	1:169:A:ARG:CA	1:169:A:ARG:C	1:170:A:VAL:N	5	1.7
(1,189)	1:153:A:ALA:C	1:154:A:GLU:N	1:154:A:GLU:CA	1:154:A:GLU:C	4	1.68
(1,140)	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	1:118:A:MET:N	3	1.67
(1,11)	1:36:A:ILE:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	2	1.65
(1,6)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:LYS:N	6	1.65
(1,255)	1:190:A:LYS:C	1:191:A:CYS:N	1:191:A:CYS:CA	1:191:A:CYS:C	10	1.62
(1,93)	1:88:A:ALA:C	1:89:A:THR:N	1:89:A:THR:CA	1:89:A:THR:C	3	1.62
(1,60)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:ASN:N	2	1.62
(1,11)	1:36:A:ILE:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	4	1.61
(1,233)	1:176:A:CYS:C	1:177:A:ALA:N	1:177:A:ALA:CA	1:177:A:ALA:C	10	1.59
(1,160)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:PRO:N	10	1.59
(1,256)	1:191:A:CYS:N	1:191:A:CYS:CA	1:191:A:CYS:C	1:192:A:LYS:N	8	1.54
(1,6)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:LYS:N	4	1.52
(1,6)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:LYS:N	2	1.45
(1,93)	1:88:A:ALA:C	1:89:A:THR:N	1:89:A:THR:CA	1:89:A:THR:C	1	1.44
(1,170)	1:138:A:THR:N	1:138:A:THR:CA	1:138:A:THR:C	1:139:A:LYS:N	2	1.43
(1,245)	1:184:A:PRO:C	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	10	1.41
(1,170)	1:138:A:THR:N	1:138:A:THR:CA	1:138:A:THR:C	1:139:A:LYS:N	6	1.39
(1,11)	1:36:A:ILE:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	7	1.37
(1,6)	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1:35:A:LYS:N	5	1.34
(1,127)	1:108:A:LYS:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	3	1.33
(1,200)	1:159:A:ILE:N	1:159:A:ILE:CA	1:159:A:ILE:C	1:160:A:ALA:N	2	1.31
(1,127)	1:108:A:LYS:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	2	1.31
(1,58)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:VAL:N	10	1.3
(1,241)	1:180:A:LYS:C	1:181:A:LYS:N	1:181:A:LYS:CA	1:181:A:LYS:C	7	1.29
(1,132)	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	1:114:A:GLU:N	9	1.28
(1,60)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:ASN:N	9	1.25
(1,188)	1:153:A:ALA:N	1:153:A:ALA:CA	1:153:A:ALA:C	1:154:A:GLU:N	2	1.24
(1,148)	1:121:A:MET:N	1:121:A:MET:CA	1:121:A:MET:C	1:122:A:MET:N	8	1.24
(1,200)	1:159:A:ILE:N	1:159:A:ILE:CA	1:159:A:ILE:C	1:160:A:ALA:N	3	1.22
(1,245)	1:184:A:PRO:C	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	3	1.18
(1,128)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:GLY:N	7	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:36:A:ILE:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	10	1.15
(1,200)	1:159:A:ILE:N	1:159:A:ILE:CA	1:159:A:ILE:C	1:160:A:ALA:N	6	1.12
(1,127)	1:108:A:LYS:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1	1.12
(1,170)	1:138:A:THR:N	1:138:A:THR:CA	1:138:A:THR:C	1:139:A:LYS:N	10	1.11
(1,255)	1:190:A:LYS:C	1:191:A:CYS:N	1:191:A:CYS:CA	1:191:A:CYS:C	6	1.07
(1,243)	1:181:A:LYS:C	1:182:A:LYS:N	1:182:A:LYS:CA	1:182:A:LYS:C	1	1.06
(1,229)	1:173:A:LYS:C	1:174:A:ASN:N	1:174:A:ASN:CA	1:174:A:ASN:C	1	1.05
(1,131)	1:112:A:SER:C	1:113:A:GLY:N	1:113:A:GLY:CA	1:113:A:GLY:C	4	1.02