



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 11:30 PM EST

PDB ID : 2MTD  
BMRB ID : 25157  
Title : Structure of Decorin Binding Protein A from strain PBr of *Borrelia garinii*  
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 : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

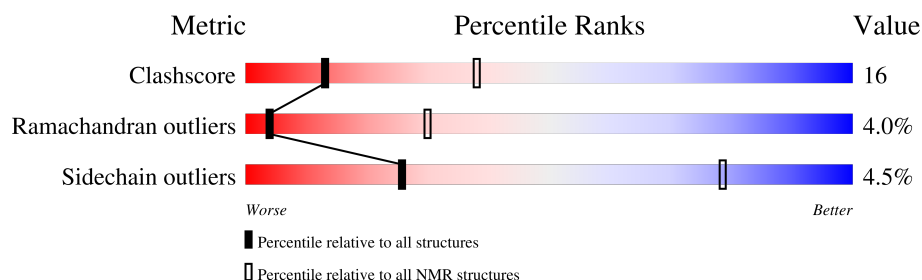
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	164	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 7 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:35-A:59, A:72-A:101, A:105-A:175 (126)	0.73	7

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 6, 7, 8, 9
2	2, 3, 5, 10
Single-model clusters	4

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2580 atoms, of which 1328 are hydrogens and 0 are deuteriums.

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

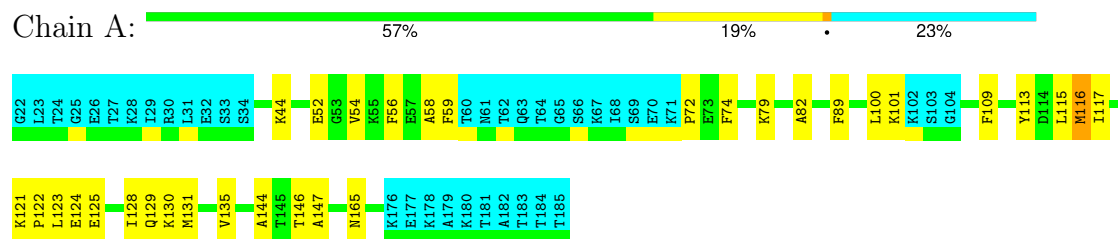
Mol	Chain	Residues	Atoms						Trace
1	A	164	Total	C	H	N	O	S	0
			2580	785	1328	214	249	4	

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Decorin binding protein A

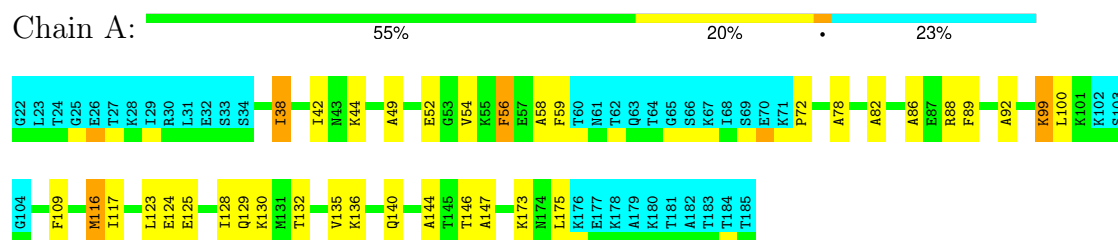


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

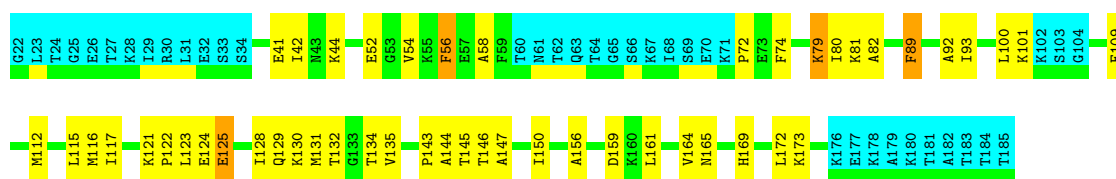
- Molecule 1: Decorin binding protein A



#### 4.2.2 Score per residue for model 2

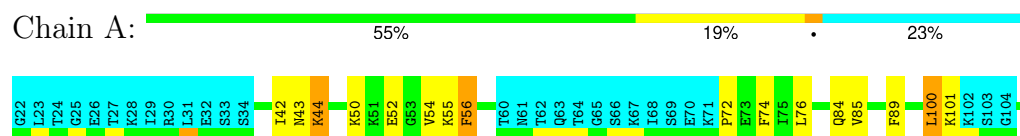
- Molecule 1: Decorin binding protein A





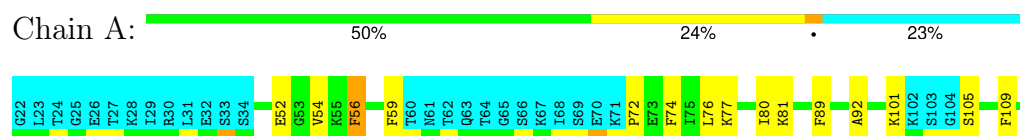
### 4.2.3 Score per residue for model 3

- Molecule 1: Decorin binding protein A



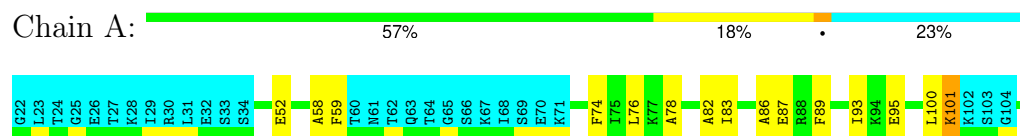
### 4.2.4 Score per residue for model 4

- Molecule 1: Decorin binding protein A



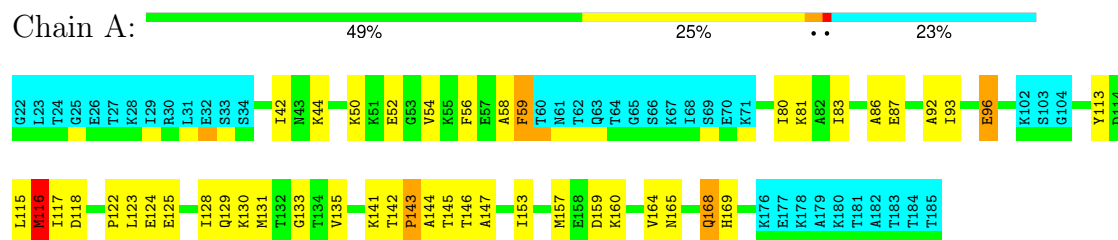
### 4.2.5 Score per residue for model 5

- Molecule 1: Decorin binding protein A



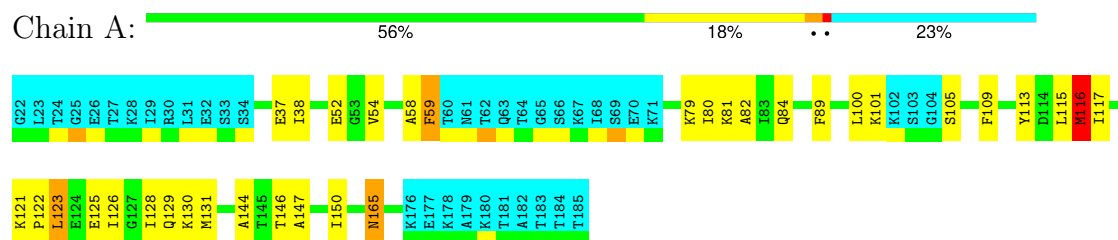
### 4.2.6 Score per residue for model 6

- Molecule 1: Decorin binding protein A



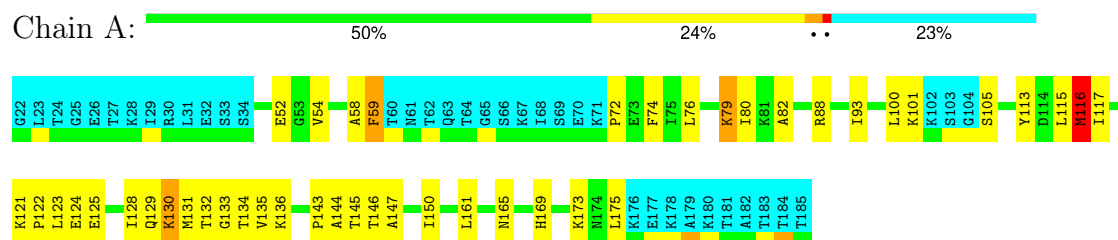
#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Decorin binding protein A



#### 4.2.8 Score per residue for model 8

- Molecule 1: Decorin binding protein A



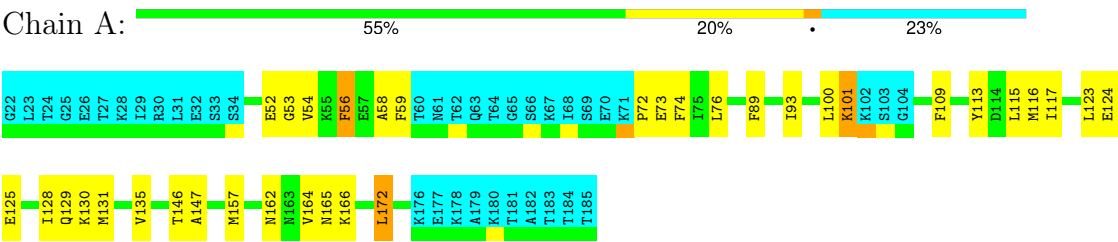
#### 4.2.9 Score per residue for model 9

- Molecule 1: Decorin binding protein A



4.2.10 Score per residue for model 10

● Molecule 1: Decorin binding protein A





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *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	1810
Number of shifts mapped to atoms	1810
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [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	973	1030	1029	32±4
All	All	9730	10300	10290	323

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ILE:O	1:A:130:LYS:N	0.67	2.28	10	10
1:A:146:THR:HG22	1:A:147:ALA:H	0.65	1.50	10	3
1:A:146:THR:HG22	1:A:147:ALA:N	0.65	2.07	10	9
1:A:38:ILE:HD12	1:A:38:ILE:H	0.62	1.55	1	1
1:A:38:ILE:H	1:A:38:ILE:CD1	0.59	2.10	1	1
1:A:128:ILE:C	1:A:130:LYS:H	0.59	2.00	10	10
1:A:169:HIS:NE2	1:A:173:LYS:NZ	0.59	2.50	2	2
1:A:100:LEU:O	1:A:100:LEU:HD13	0.58	1.97	5	2
1:A:116:MET:SD	1:A:116:MET:N	0.57	2.77	6	5
1:A:38:ILE:HD12	1:A:38:ILE:N	0.57	2.14	1	1
1:A:161:LEU:C	1:A:161:LEU:HD12	0.56	2.21	5	2
1:A:168:GLN:NE2	1:A:169:HIS:ND1	0.56	2.52	4	1
1:A:54:VAL:O	1:A:56:PHE:CE1	0.55	2.60	1	6
1:A:109:PHE:CZ	1:A:144:ALA:HB1	0.54	2.38	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:MET:N	1:A:131:MET:SD	0.54	2.80	3	6
1:A:168:GLN:NE2	1:A:169:HIS:CG	0.53	2.76	4	1
1:A:78:ALA:O	1:A:82:ALA:N	0.53	2.41	5	2
1:A:145:THR:HG22	1:A:145:THR:O	0.53	2.03	2	1
1:A:93:ILE:HD12	1:A:93:ILE:N	0.53	2.18	5	5
1:A:52:GLU:C	1:A:54:VAL:H	0.52	2.07	10	9
1:A:175:LEU:N	1:A:175:LEU:HD22	0.52	2.19	8	1
1:A:109:PHE:CZ	1:A:144:ALA:CB	0.52	2.92	1	4
1:A:143:PRO:C	1:A:145:THR:H	0.52	2.07	6	4
1:A:123:LEU:C	1:A:123:LEU:HD23	0.51	2.25	8	2
1:A:89:PHE:O	1:A:92:ALA:N	0.51	2.43	1	3
1:A:115:LEU:O	1:A:117:ILE:N	0.51	2.43	3	8
1:A:123:LEU:O	1:A:125:GLU:N	0.51	2.44	3	9
1:A:99:LYS:CD	1:A:99:LYS:N	0.50	2.74	1	1
1:A:169:HIS:CD2	1:A:173:LYS:NZ	0.50	2.78	2	2
1:A:128:ILE:C	1:A:130:LYS:N	0.50	2.65	5	10
1:A:74:PHE:C	1:A:74:PHE:CD1	0.50	2.85	2	1
1:A:74:PHE:O	1:A:77:LYS:N	0.50	2.44	4	1
1:A:52:GLU:O	1:A:54:VAL:N	0.49	2.45	10	5
1:A:52:GLU:OE1	1:A:74:PHE:CD1	0.49	2.65	10	2
1:A:146:THR:CG2	1:A:147:ALA:N	0.49	2.76	10	8
1:A:165:ASN:OD1	1:A:169:HIS:ND1	0.49	2.46	6	1
1:A:132:THR:O	1:A:134:THR:N	0.49	2.46	8	1
1:A:128:ILE:O	1:A:128:ILE:CG2	0.49	2.60	3	10
1:A:44:LYS:HZ3	1:A:44:LYS:HB3	0.49	1.67	3	1
1:A:135:VAL:HG23	1:A:136:LYS:N	0.48	2.23	8	1
1:A:100:LEU:HD13	1:A:100:LEU:C	0.48	2.28	5	1
1:A:175:LEU:N	1:A:175:LEU:CD2	0.48	2.76	8	1
1:A:79:LYS:O	1:A:82:ALA:N	0.48	2.46	9	4
1:A:169:HIS:CD2	1:A:173:LYS:HZ3	0.48	2.27	2	1
1:A:76:LEU:HD22	1:A:76:LEU:N	0.48	2.22	10	3
1:A:109:PHE:CE2	1:A:144:ALA:O	0.48	2.67	5	1
1:A:56:PHE:CD1	1:A:56:PHE:N	0.48	2.81	4	5
1:A:93:ILE:N	1:A:93:ILE:CD1	0.48	2.77	5	4
1:A:115:LEU:C	1:A:117:ILE:N	0.48	2.67	3	8
1:A:132:THR:O	1:A:135:VAL:HG22	0.48	2.08	8	1
1:A:168:GLN:HE21	1:A:169:HIS:N	0.47	2.07	4	1
1:A:44:LYS:CB	1:A:44:LYS:NZ	0.47	2.77	3	1
1:A:124:GLU:OE2	1:A:129:GLN:NE2	0.47	2.48	5	1
1:A:159:ASP:N	1:A:159:ASP:OD1	0.47	2.46	2	1
1:A:164:VAL:HG23	1:A:165:ASN:N	0.47	2.24	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:LEU:HD22	1:A:172:LEU:N	0.47	2.24	2	1
1:A:147:ALA:O	1:A:150:ILE:N	0.47	2.47	7	4
1:A:159:ASP:OD1	1:A:160:LYS:N	0.47	2.48	6	1
1:A:175:LEU:HD12	1:A:175:LEU:N	0.47	2.25	1	2
1:A:76:LEU:N	1:A:76:LEU:CD2	0.47	2.77	10	3
1:A:146:THR:CG2	1:A:147:ALA:H	0.47	2.21	10	1
1:A:109:PHE:O	1:A:112:MET:N	0.46	2.47	2	1
1:A:72:PRO:O	1:A:74:PHE:N	0.46	2.48	10	1
1:A:84:GLN:CG	1:A:85:VAL:N	0.46	2.79	3	1
1:A:42:ILE:C	1:A:44:LYS:N	0.46	2.69	3	5
1:A:172:LEU:N	1:A:172:LEU:CD2	0.46	2.79	2	1
1:A:54:VAL:HG12	1:A:55:LYS:N	0.46	2.25	3	1
1:A:42:ILE:O	1:A:44:LYS:N	0.46	2.49	3	1
1:A:84:GLN:NE2	1:A:165:ASN:OD1	0.46	2.49	7	1
1:A:131:MET:SD	1:A:161:LEU:CD2	0.46	3.04	2	1
1:A:168:GLN:NE2	1:A:169:HIS:N	0.46	2.64	4	1
1:A:123:LEU:C	1:A:125:GLU:N	0.46	2.69	3	10
1:A:59:PHE:CD1	1:A:59:PHE:O	0.45	2.69	10	4
1:A:108:ALA:O	1:A:112:MET:SD	0.45	2.74	3	2
1:A:80:ILE:HG22	1:A:168:GLN:NE2	0.45	2.26	4	1
1:A:123:LEU:HD21	1:A:128:ILE:HB	0.45	1.87	8	2
1:A:132:THR:C	1:A:134:THR:N	0.45	2.69	8	1
1:A:135:VAL:CG2	1:A:157:MET:SD	0.45	3.05	10	2
1:A:172:LEU:HD13	1:A:172:LEU:O	0.45	2.12	10	1
1:A:166:LYS:O	1:A:170:ASP:N	0.45	2.48	4	1
1:A:113:TYR:O	1:A:116:MET:N	0.44	2.49	5	5
1:A:164:VAL:O	1:A:168:GLN:NE2	0.44	2.50	6	1
1:A:86:ALA:C	1:A:88:ARG:N	0.44	2.71	1	1
1:A:132:THR:O	1:A:135:VAL:HG12	0.44	2.12	2	2
1:A:130:LYS:O	1:A:133:GLY:N	0.44	2.45	6	1
1:A:83:ILE:O	1:A:86:ALA:HB3	0.44	2.12	5	2
1:A:80:ILE:CG1	1:A:81:LYS:N	0.44	2.81	6	4
1:A:80:ILE:HG13	1:A:81:LYS:N	0.44	2.28	4	3
1:A:76:LEU:O	1:A:80:ILE:HD12	0.44	2.13	8	1
1:A:136:LYS:O	1:A:140:GLN:OE1	0.44	2.36	1	1
1:A:72:PRO:C	1:A:74:PHE:N	0.44	2.71	2	4
1:A:37:GLU:CG	1:A:38:ILE:N	0.44	2.80	7	1
1:A:100:LEU:O	1:A:101:LYS:C	0.43	2.57	5	3
1:A:96:GLU:OE2	1:A:112:MET:SD	0.43	2.76	9	1
1:A:54:VAL:CG1	1:A:55:LYS:N	0.43	2.82	3	1
1:A:140:GLN:N	1:A:140:GLN:CD	0.43	2.72	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:ILE:O	1:A:157:MET:SD	0.43	2.77	4	2
1:A:165:ASN:OD1	1:A:166:LYS:N	0.43	2.50	10	1
1:A:117:ILE:HD12	1:A:117:ILE:H	0.43	1.74	1	1
1:A:109:PHE:CD2	1:A:144:ALA:O	0.43	2.72	5	1
1:A:80:ILE:HD12	1:A:80:ILE:H	0.43	1.73	8	1
1:A:74:PHE:CD1	1:A:74:PHE:C	0.43	2.92	10	1
1:A:140:GLN:OE1	1:A:140:GLN:N	0.43	2.51	1	1
1:A:132:THR:O	1:A:135:VAL:CG1	0.42	2.67	2	1
1:A:52:GLU:C	1:A:54:VAL:N	0.42	2.73	10	1
1:A:132:THR:O	1:A:135:VAL:N	0.42	2.50	4	1
1:A:109:PHE:CZ	1:A:113:TYR:CG	0.42	3.07	10	1
1:A:49:ALA:O	1:A:56:PHE:CE1	0.42	2.72	1	1
1:A:92:ALA:O	1:A:96:GLU:OE2	0.42	2.38	6	1
1:A:165:ASN:OD1	1:A:169:HIS:CE1	0.42	2.72	6	1
1:A:165:ASN:ND2	1:A:165:ASN:C	0.42	2.73	7	1
1:A:121:LYS:N	1:A:122:PRO:HD2	0.42	2.30	3	1
1:A:134:THR:O	1:A:137:GLU:N	0.42	2.52	9	1
1:A:121:LYS:CB	1:A:122:PRO:CD	0.42	2.98	7	5
1:A:128:ILE:O	1:A:128:ILE:HG22	0.42	2.15	3	2
1:A:56:PHE:O	1:A:59:PHE:N	0.42	2.49	4	1
1:A:121:LYS:O	1:A:124:GLU:CG	0.42	2.67	9	1
1:A:157:MET:SD	1:A:157:MET:N	0.41	2.93	4	1
1:A:109:PHE:CE2	1:A:150:ILE:HD11	0.41	2.50	2	1
1:A:142:THR:OG1	1:A:153:ILE:CG1	0.41	2.68	6	1
1:A:175:LEU:N	1:A:175:LEU:CD1	0.41	2.83	9	1
1:A:162:ASN:O	1:A:165:ASN:OD1	0.41	2.39	10	1
1:A:139:ALA:O	1:A:142:THR:O	0.41	2.38	4	1
1:A:89:PHE:O	1:A:93:ILE:HD13	0.41	2.16	5	1
1:A:143:PRO:C	1:A:145:THR:N	0.41	2.74	6	1
1:A:115:LEU:N	1:A:115:LEU:CD2	0.41	2.83	8	1
1:A:54:VAL:O	1:A:56:PHE:CD1	0.41	2.74	1	2
1:A:78:ALA:O	1:A:82:ALA:CB	0.41	2.69	5	1
1:A:135:VAL:CG2	1:A:136:LYS:N	0.41	2.84	8	1
1:A:161:LEU:C	1:A:161:LEU:CD1	0.41	2.89	5	1
1:A:118:ASP:O	1:A:122:PRO:CD	0.41	2.69	6	1
1:A:123:LEU:CD2	1:A:126:ILE:HG22	0.41	2.45	7	1
1:A:161:LEU:O	1:A:165:ASN:CG	0.41	2.60	8	1
1:A:150:ILE:HA	1:A:153:ILE:HD12	0.41	1.92	9	1
1:A:164:VAL:CG2	1:A:165:ASN:N	0.41	2.84	10	1
1:A:74:PHE:C	1:A:76:LEU:N	0.41	2.74	4	1
1:A:109:PHE:CZ	1:A:113:TYR:CD1	0.40	3.09	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LYS:CG	1:A:137:GLU:N	0.40	2.83	9	1
1:A:168:GLN:HE21	1:A:168:GLN:C	0.40	2.20	4	1
1:A:156:ALA:O	1:A:159:ASP:OD1	0.40	2.40	2	1
1:A:86:ALA:O	1:A:88:ARG:N	0.40	2.55	1	1
1:A:115:LEU:O	1:A:119:VAL:HG12	0.40	2.17	4	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	126/164 (77%)	107±3 (85±2%)	14±3 (11±3%)	5±1 (4±1%)	4	30
All	All	1260/1640 (77%)	1068 (85%)	141 (11%)	51 (4%)	4	30

All 13 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	129	GLN	10
1	A	124	GLU	9
1	A	116	MET	8
1	A	101	LYS	6
1	A	59	PHE	5
1	A	144	ALA	4
1	A	79	LYS	2
1	A	105	SER	2
1	A	43	ASN	1
1	A	143	PRO	1
1	A	133	GLY	1
1	A	53	GLY	1
1	A	73	GLU	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	102/134 (76%)	97±1 (95±1%)	5±1 (5±1%)	26 78
All	All	1020/1340 (76%)	974 (95%)	46 (5%)	26 78

All 25 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	56	PHE	6
1	A	116	MET	5
1	A	100	LEU	4
1	A	89	PHE	4
1	A	50	LYS	2
1	A	130	LYS	2
1	A	168	GLN	2
1	A	87	GLU	2
1	A	131	MET	2
1	A	88	ARG	2
1	A	38	ILE	1
1	A	99	LYS	1
1	A	41	GLU	1
1	A	125	GLU	1
1	A	134	THR	1
1	A	44	LYS	1
1	A	155	GLN	1
1	A	175	LEU	1
1	A	95	GLU	1
1	A	96	GLU	1
1	A	141	LYS	1
1	A	123	LEU	1
1	A	165	ASN	1
1	A	59	PHE	1
1	A	172	LEU	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

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 82% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *PBr\_list*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1810
Number of shifts mapped to atoms	1810
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	163	$1.57 \pm 0.16$	Should be checked
$^{13}\text{C}_\beta$	154	$3.10 \pm 0.10$	Should be checked
$^{13}\text{C}'$	147	$-0.42 \pm 0.37$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	155	$0.34 \pm 0.28$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1427 atoms were assigned a chemical shift out of a possible 1730. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	608/629 (97%)	249/254 (98%)	240/252 (95%)	119/123 (97%)
Sidechain	795/1034 (77%)	510/670 (76%)	285/328 (87%)	0/36 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	24/67 (36%)	12/33 (36%)	12/32 (38%)	0/2 (0%)
Overall	1427/1730 (82%)	771/957 (81%)	537/612 (88%)	119/161 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1810 atoms were assigned a chemical shift out of a possible 2207. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	788/823 (96%)	323/334 (97%)	310/328 (95%)	155/161 (96%)
Sidechain	998/1317 (76%)	638/851 (75%)	360/418 (86%)	0/48 (0%)
Aromatic	24/67 (36%)	12/33 (36%)	12/32 (38%)	0/2 (0%)
Overall	1810/2207 (82%)	973/1218 (80%)	682/778 (88%)	155/211 (73%)

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

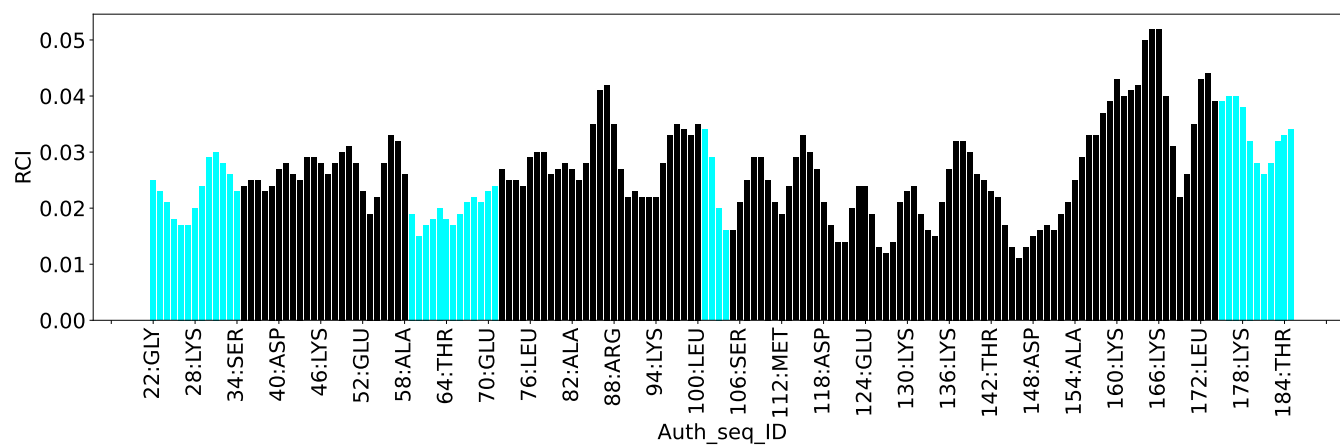
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	GLY	C	184.89	164.92 – 182.89	6.1

#### 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	1524
Intra-residue ( $ i-j =0$ )	437
Sequential ( $ i-j =1$ )	518
Medium range ( $ i-j >1$ and $ i-j <5$ )	317
Long range ( $ i-j \geq 5$ )	252
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	280
Number of unmapped restraints	0
Number of restraints per residue	11.0
Number of long range restraints per residue <sup>1</sup>	1.5

<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)	48.3	0.2
0.2-0.5 (Medium)	57.9	0.5
>0.5 (Large)	1.4	1.25

### 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)	24.1	8.69
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

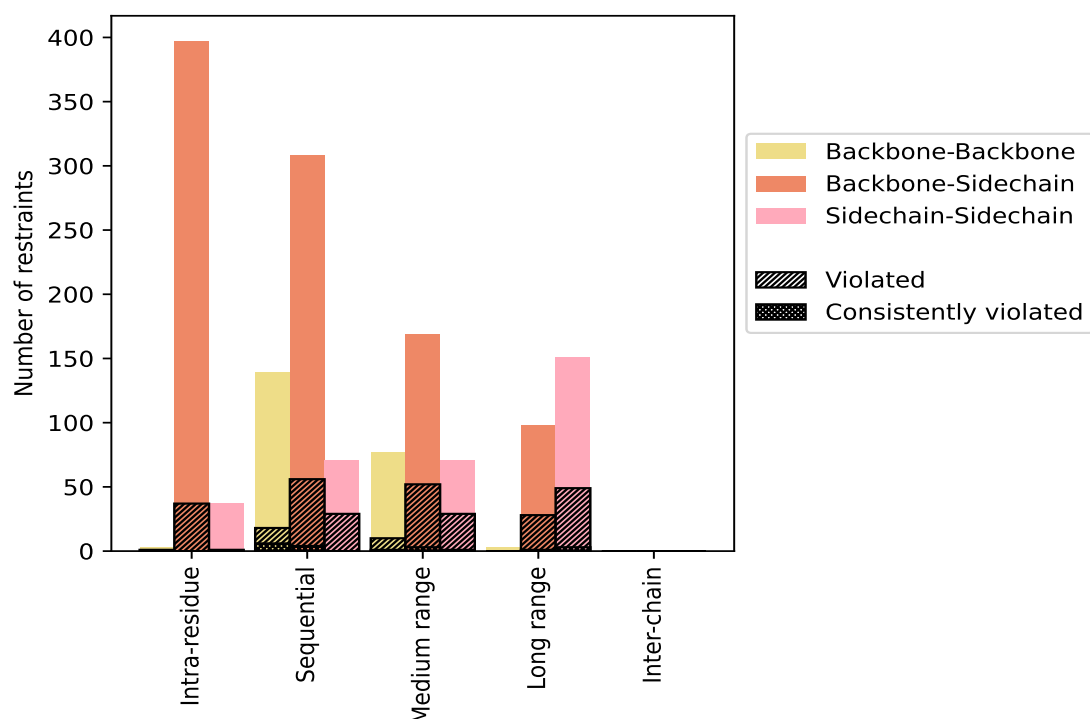
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <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>437</b>	<b>28.7</b>	<b>39</b>	<b>8.9</b>	<b>2.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	3	0.2	1	33.3	0.1	0	0.0	0.0
Backbone-Sidechain	397	26.0	37	9.3	2.4	0	0.0	0.0
Sidechain-Sidechain	37	2.4	1	2.7	0.1	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>518</b>	<b>34.0</b>	<b>103</b>	<b>19.9</b>	<b>6.8</b>	<b>10</b>	<b>1.9</b>	<b>0.7</b>
Backbone-Backbone	139	9.1	18	12.9	1.2	6	4.3	0.4
Backbone-Sidechain	308	20.2	56	18.2	3.7	4	1.3	0.3
Sidechain-Sidechain	71	4.7	29	40.8	1.9	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>317</b>	<b>20.8</b>	<b>91</b>	<b>28.7</b>	<b>6.0</b>	<b>5</b>	<b>1.6</b>	<b>0.3</b>
Backbone-Backbone	77	5.1	10	13.0	0.7	1	1.3	0.1
Backbone-Sidechain	169	11.1	52	30.8	3.4	3	1.8	0.2
Sidechain-Sidechain	71	4.7	29	40.8	1.9	1	1.4	0.1
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>252</b>	<b>16.5</b>	<b>77</b>	<b>30.6</b>	<b>5.1</b>	<b>4</b>	<b>1.6</b>	<b>0.3</b>
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	98	6.4	28	28.6	1.8	1	1.0	0.1
Sidechain-Sidechain	151	9.9	49	32.5	3.2	3	2.0	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>1524</b>	<b>100.0</b>	<b>310</b>	<b>20.3</b>	<b>20.3</b>	<b>19</b>	<b>1.2</b>	<b>1.2</b>
Backbone-Backbone	222	14.6	29	13.1	1.9	7	3.2	0.5
Backbone-Sidechain	972	63.8	173	17.8	11.4	8	0.8	0.5
Sidechain-Sidechain	330	21.7	108	32.7	7.1	4	1.2	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 disulfied bonds are counted in their appropriate category on the x-axis

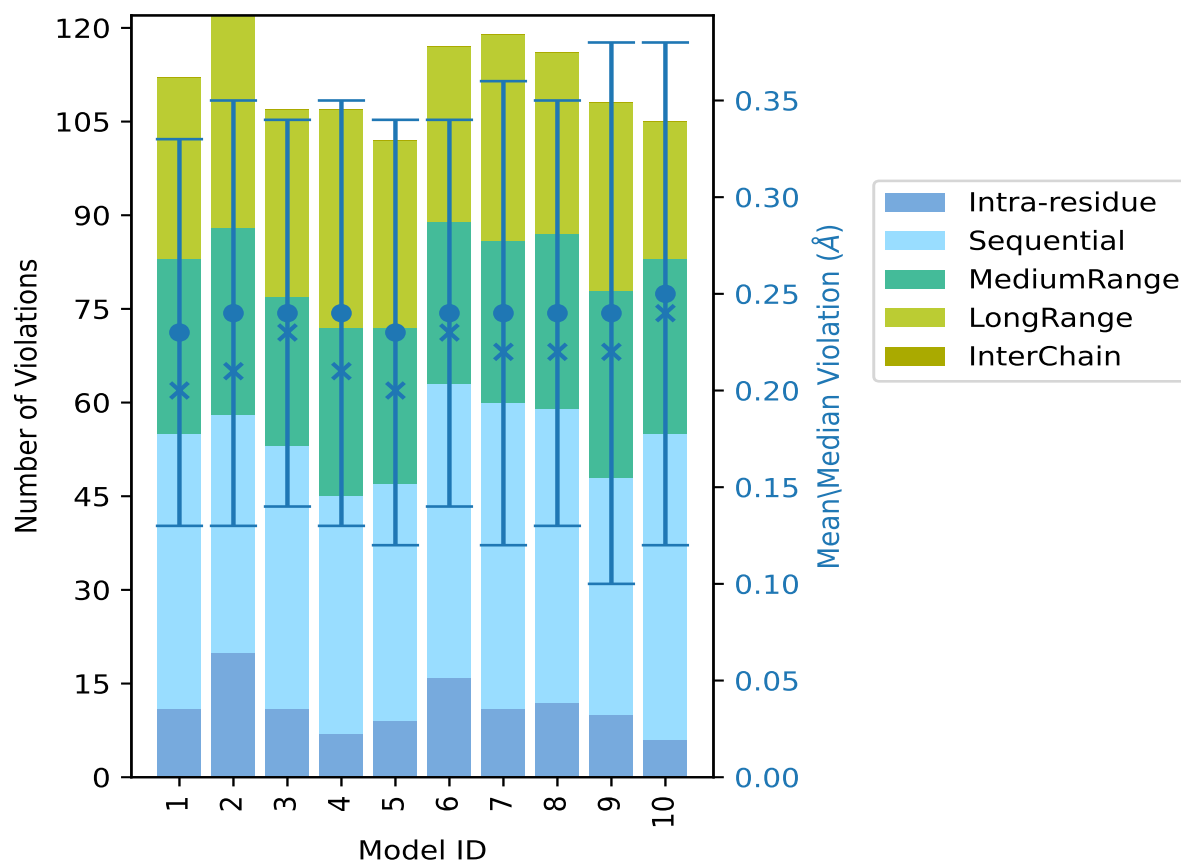
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	11	44	28	29	0	112	0.23	0.57	0.1	0.2
2	20	38	30	34	0	122	0.24	0.66	0.11	0.21
3	11	42	24	30	0	107	0.24	0.6	0.1	0.23
4	7	38	27	35	0	107	0.24	0.69	0.11	0.21
5	9	38	25	30	0	102	0.23	0.7	0.11	0.2
6	16	47	26	28	0	117	0.24	0.61	0.1	0.23
7	11	49	26	33	0	119	0.24	0.89	0.12	0.22
8	12	47	28	29	0	116	0.24	0.76	0.11	0.22
9	10	38	30	30	0	108	0.24	1.25	0.14	0.22
10	6	49	28	22	0	105	0.25	0.99	0.13	0.24

<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, 1214(IR:398, SQ:415, MR:226, LR:175, 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>	%
14	28	34	19	0	95	1	10.0
10	13	17	16	0	56	2	20.0
3	10	13	9	0	35	3	30.0

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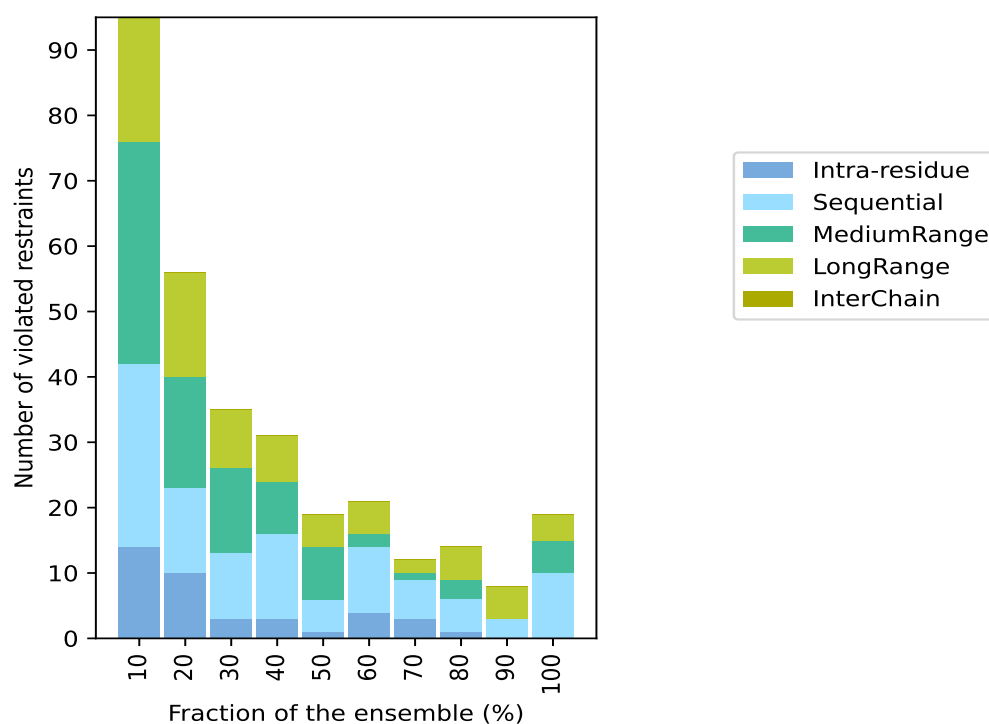
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
3	13	8	7	0	31	4	40.0
1	5	8	5	0	19	5	50.0
4	10	2	5	0	21	6	60.0
3	6	1	2	0	12	7	70.0
1	5	3	5	0	14	8	80.0
0	3	0	5	0	8	9	90.0
0	10	5	4	0	19	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 ⓘ

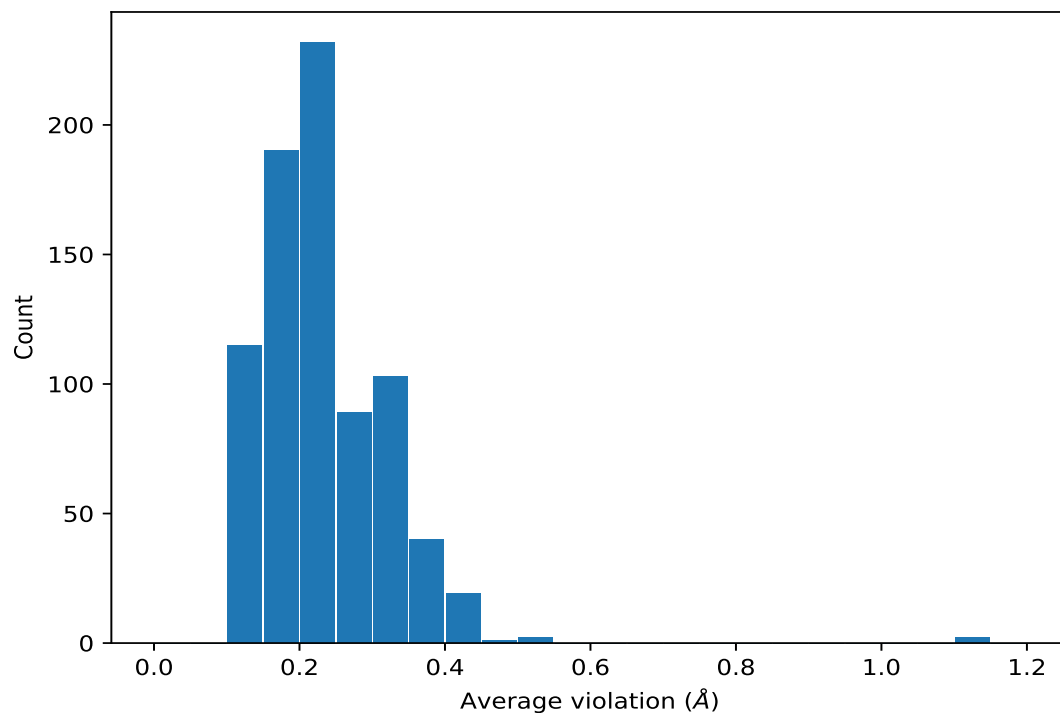


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	10	0.53	0.15	0.48
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	10	0.53	0.15	0.48
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	10	0.41	0.12	0.42
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	10	0.41	0.12	0.42
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	10	0.41	0.12	0.42
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	10	0.38	0.1	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	10	0.38	0.1	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	10	0.38	0.1	0.4
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	10	0.37	0.07	0.38
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	10	0.35	0.02	0.36
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	10	0.35	0.08	0.36
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	10	0.35	0.08	0.36
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	10	0.35	0.08	0.36
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	10	0.33	0.07	0.34
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	10	0.33	0.07	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	10	0.33	0.07	0.34
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	10	0.33	0.07	0.34
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	10	0.33	0.07	0.34
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	10	0.33	0.07	0.34
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	10	0.33	0.07	0.34
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	10	0.33	0.07	0.34
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	10	0.33	0.07	0.34
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	10	0.32	0.07	0.32
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	10	0.3	0.01	0.3
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	10	0.29	0.08	0.27
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	10	0.29	0.08	0.27
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	10	0.29	0.08	0.27
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	10	0.28	0.02	0.28
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	10	0.28	0.02	0.28
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	10	0.28	0.02	0.28
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	10	0.27	0.1	0.22
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	10	0.27	0.06	0.26
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	10	0.27	0.06	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	10	0.27	0.06	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	10	0.27	0.06	0.24
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	10	0.25	0.06	0.27
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	10	0.25	0.06	0.27
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	10	0.25	0.03	0.25
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	10	0.25	0.03	0.25
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	10	0.21	0.04	0.22
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	10	0.18	0.07	0.17
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	10	0.18	0.07	0.17
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	10	0.18	0.07	0.17
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	10	0.16	0.05	0.15
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	10	0.16	0.05	0.15
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	9	0.36	0.05	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	9	0.36	0.05	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	9	0.36	0.05	0.35
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	9	0.31	0.11	0.28
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	9	0.31	0.11	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	9	0.31	0.11	0.28
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	9	0.29	0.11	0.27
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	9	0.29	0.11	0.27
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	9	0.29	0.11	0.27
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	9	0.25	0.07	0.27
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	9	0.25	0.07	0.27
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	9	0.22	0.08	0.21
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	9	0.22	0.08	0.21
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	9	0.22	0.08	0.21
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	9	0.22	0.05	0.2
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	9	0.22	0.05	0.2
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	9	0.22	0.09	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	9	0.22	0.09	0.21
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	9	0.2	0.02	0.2
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	8	0.37	0.1	0.37
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	8	0.37	0.1	0.37
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	8	0.37	0.1	0.37
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	8	0.37	0.1	0.37
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	8	0.37	0.1	0.37
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	8	0.37	0.1	0.37
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	8	0.33	0.04	0.33
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	8	0.31	0.09	0.34
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	8	0.31	0.09	0.34
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	8	0.31	0.09	0.34
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	8	0.31	0.09	0.34
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	8	0.31	0.09	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	8	0.31	0.09	0.34
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	8	0.27	0.08	0.32
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	8	0.27	0.1	0.25
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	8	0.27	0.1	0.25
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	8	0.27	0.1	0.25
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	8	0.26	0.03	0.25
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	8	0.26	0.03	0.25
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	8	0.24	0.05	0.22
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	8	0.24	0.05	0.22
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	8	0.24	0.05	0.22
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	8	0.24	0.05	0.22
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	8	0.24	0.05	0.22
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	8	0.24	0.05	0.22
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	8	0.23	0.07	0.26
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	8	0.23	0.07	0.26
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	8	0.23	0.07	0.26
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	8	0.23	0.07	0.26
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	8	0.22	0.07	0.21
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	8	0.22	0.07	0.21
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	8	0.22	0.07	0.21
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	8	0.22	0.07	0.21
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	8	0.22	0.07	0.21
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	8	0.22	0.07	0.21
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	8	0.22	0.06	0.22
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	8	0.22	0.06	0.22
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	8	0.22	0.06	0.22
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	8	0.22	0.06	0.22
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	8	0.22	0.06	0.22
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	8	0.22	0.06	0.22
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	8	0.21	0.08	0.2
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	8	0.21	0.06	0.2
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	8	0.21	0.06	0.2
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	8	0.21	0.06	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	8	0.2	0.03	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	8	0.2	0.03	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	8	0.2	0.03	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	8	0.2	0.03	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	8	0.2	0.03	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	8	0.2	0.03	0.2
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	8	0.13	0.02	0.13
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	7	0.35	0.08	0.32
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	7	0.35	0.08	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	7	0.33	0.12	0.26
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	7	0.33	0.12	0.26
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	7	0.33	0.12	0.26
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	7	0.33	0.12	0.26
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	7	0.33	0.12	0.26
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	7	0.33	0.12	0.26
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	7	0.32	0.11	0.36
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	7	0.29	0.11	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	7	0.29	0.11	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	7	0.29	0.11	0.29
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	7	0.25	0.07	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	7	0.25	0.07	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	7	0.25	0.07	0.28
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	7	0.25	0.03	0.24
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	7	0.24	0.05	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	7	0.24	0.05	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	7	0.24	0.05	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	7	0.24	0.05	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	7	0.24	0.05	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	7	0.24	0.05	0.23
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	7	0.23	0.11	0.19
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	7	0.23	0.11	0.19
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	7	0.23	0.06	0.24
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	7	0.18	0.05	0.17
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	7	0.18	0.05	0.17
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	7	0.16	0.01	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	7	0.16	0.01	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	7	0.16	0.01	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	7	0.16	0.01	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	7	0.16	0.01	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	7	0.16	0.01	0.16
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	7	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	7	0.12	0.02	0.12
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	7	0.12	0.02	0.12
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB2	6	0.37	0.19	0.29
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB3	6	0.37	0.19	0.29
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB2	6	0.37	0.19	0.29
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB3	6	0.37	0.19	0.29
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG21	6	0.3	0.11	0.34
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG22	6	0.3	0.11	0.34
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG23	6	0.3	0.11	0.34
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD11	6	0.3	0.09	0.33
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD12	6	0.3	0.09	0.33
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD13	6	0.3	0.09	0.33
(1,200)	1:29:A:ILE:HB	1:30:A:ARG:HA	6	0.26	0.12	0.24
(1,393)	1:88:A:ARG:H	1:88:A:ARG:HG3	6	0.26	0.04	0.26
(1,709)	1:98:A:GLU:H	1:99:A:LYS:HD3	6	0.24	0.06	0.26
(1,207)	1:90:A:VAL:HG21	1:154:A:ALA:HA	6	0.23	0.1	0.21
(1,207)	1:90:A:VAL:HG22	1:154:A:ALA:HA	6	0.23	0.1	0.21
(1,207)	1:90:A:VAL:HG23	1:154:A:ALA:HA	6	0.23	0.1	0.21
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD21	6	0.23	0.03	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD22	6	0.23	0.03	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD23	6	0.23	0.03	0.23
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG11	6	0.22	0.05	0.22
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG12	6	0.22	0.05	0.22
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG13	6	0.22	0.05	0.22
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG21	6	0.22	0.05	0.22
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG22	6	0.22	0.05	0.22
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG23	6	0.22	0.05	0.22
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB1	6	0.2	0.07	0.18
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB2	6	0.2	0.07	0.18
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB3	6	0.2	0.07	0.18
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB1	6	0.2	0.07	0.18
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB2	6	0.2	0.07	0.18
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB3	6	0.2	0.07	0.18
(1,83)	1:52:A:GLU:H	1:52:A:GLU:HG2	6	0.19	0.01	0.18
(1,551)	1:68:A:ILE:HA	1:69:A:SER:H	6	0.18	0.02	0.2
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB2	6	0.18	0.05	0.19
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB3	6	0.18	0.05	0.19
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG21	6	0.18	0.05	0.18
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG22	6	0.18	0.05	0.18
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG23	6	0.18	0.05	0.18
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD1	6	0.18	0.06	0.15
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD2	6	0.18	0.06	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG12	6	0.18	0.04	0.17
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG13	6	0.18	0.04	0.17
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG2	6	0.16	0.01	0.16
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG3	6	0.16	0.01	0.16
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE1	6	0.16	0.04	0.16
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE2	6	0.16	0.04	0.16
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE3	6	0.16	0.04	0.16
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE1	6	0.16	0.04	0.16
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE2	6	0.16	0.04	0.16
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE3	6	0.16	0.04	0.16
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB1	6	0.15	0.03	0.15
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB2	6	0.15	0.03	0.15
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB3	6	0.15	0.03	0.15
(1,533)	1:49:A:ALA:H	1:50:A:LYS:HA	6	0.14	0.03	0.13
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD11	6	0.12	0.01	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD12	6	0.12	0.01	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD13	6	0.12	0.01	0.11
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB2	5	0.42	0.08	0.44
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB3	5	0.42	0.08	0.44
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB2	5	0.42	0.08	0.44
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB3	5	0.42	0.08	0.44
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB2	5	0.42	0.08	0.44
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB3	5	0.42	0.08	0.44
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG2	5	0.38	0.1	0.38
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG3	5	0.38	0.1	0.38
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG2	5	0.38	0.1	0.38
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG3	5	0.38	0.1	0.38
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG2	5	0.38	0.1	0.38
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG3	5	0.38	0.1	0.38
(1,1104)	1:51:A:LYS:HD2	1:52:A:GLU:H	5	0.36	0.07	0.39
(1,1104)	1:51:A:LYS:HD3	1:52:A:GLU:H	5	0.36	0.07	0.39
(1,1311)	1:101:A:LYS:HD2	1:103:A:SER:H	5	0.31	0.07	0.34
(1,1311)	1:101:A:LYS:HD3	1:103:A:SER:H	5	0.31	0.07	0.34
(1,710)	1:98:A:GLU:H	1:99:A:LYS:HD2	5	0.27	0.02	0.26
(1,122)	1:83:A:ILE:HD11	1:85:A:VAL:H	5	0.26	0.13	0.32
(1,122)	1:83:A:ILE:HD12	1:85:A:VAL:H	5	0.26	0.13	0.32
(1,122)	1:83:A:ILE:HD13	1:85:A:VAL:H	5	0.26	0.13	0.32
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD2	5	0.25	0.1	0.2
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD3	5	0.25	0.1	0.2
(1,394)	1:88:A:ARG:H	1:88:A:ARG:HG2	5	0.25	0.07	0.28
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE1	5	0.24	0.12	0.2
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE2	5	0.24	0.12	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG12	5	0.24	0.04	0.23
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG13	5	0.24	0.04	0.23
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG12	5	0.24	0.04	0.23
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG13	5	0.24	0.04	0.23
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG12	5	0.24	0.04	0.23
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG13	5	0.24	0.04	0.23
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG12	5	0.22	0.04	0.23
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG13	5	0.22	0.04	0.23
(1,69)	1:88:A:ARG:HD3	1:92:A:ALA:H	5	0.22	0.07	0.24
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD11	5	0.2	0.06	0.19
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD12	5	0.2	0.06	0.19
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD13	5	0.2	0.06	0.19
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG21	5	0.19	0.06	0.18
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG22	5	0.19	0.06	0.18
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG23	5	0.19	0.06	0.18
(1,765)	1:150:A:ILE:HG21	1:153:A:ILE:H	5	0.19	0.08	0.14
(1,765)	1:150:A:ILE:HG22	1:153:A:ILE:H	5	0.19	0.08	0.14
(1,765)	1:150:A:ILE:HG23	1:153:A:ILE:H	5	0.19	0.08	0.14
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE1	5	0.19	0.07	0.15
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE2	5	0.19	0.07	0.15
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE3	5	0.19	0.07	0.15
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE1	5	0.19	0.07	0.15
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE2	5	0.19	0.07	0.15
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE3	5	0.19	0.07	0.15
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG21	5	0.18	0.04	0.19
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG22	5	0.18	0.04	0.19
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG23	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG2	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG3	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG2	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG3	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG2	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG3	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG2	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG3	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG2	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG3	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG2	5	0.18	0.04	0.19
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG3	5	0.18	0.04	0.19
(1,257)	1:59:A:PHE:HB2	1:60:A:THR:HA	5	0.14	0.01	0.14
(1,535)	1:62:A:THR:HB	1:63:A:GLN:H	4	0.48	0.08	0.44
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG21	4	0.4	0.03	0.41

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG22	4	0.4	0.03	0.41
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG23	4	0.4	0.03	0.41
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG21	4	0.4	0.03	0.41
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG22	4	0.4	0.03	0.41
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG23	4	0.4	0.03	0.41
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG21	4	0.4	0.03	0.41
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG22	4	0.4	0.03	0.41
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG23	4	0.4	0.03	0.41
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG12	4	0.36	0.13	0.4
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG13	4	0.36	0.13	0.4
(1,1306)	1:101:A:LYS:HB2	1:147:A:ALA:HA	4	0.34	0.08	0.32
(1,1306)	1:101:A:LYS:HB3	1:147:A:ALA:HA	4	0.34	0.08	0.32
(1,794)	1:68:A:ILE:HD11	1:69:A:SER:H	4	0.33	0.05	0.36
(1,794)	1:68:A:ILE:HD12	1:69:A:SER:H	4	0.33	0.05	0.36
(1,794)	1:68:A:ILE:HD13	1:69:A:SER:H	4	0.33	0.05	0.36
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG21	4	0.32	0.01	0.32
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG22	4	0.32	0.01	0.32
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG23	4	0.32	0.01	0.32
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	4	0.3	0.02	0.3
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	4	0.3	0.02	0.3
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	4	0.3	0.02	0.3
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	4	0.3	0.02	0.3
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	4	0.3	0.02	0.3
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	4	0.3	0.02	0.3
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE2	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE3	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE2	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE3	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE2	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE3	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE2	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE3	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE2	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE3	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE2	4	0.3	0.08	0.29
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE3	4	0.3	0.08	0.29
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD11	4	0.27	0.04	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD12	4	0.27	0.04	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD13	4	0.27	0.04	0.25
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE1	4	0.24	0.1	0.24
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE2	4	0.24	0.1	0.24
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE3	4	0.24	0.1	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE1	4	0.24	0.1	0.24
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE2	4	0.24	0.1	0.24
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE3	4	0.24	0.1	0.24
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD2	4	0.23	0.12	0.21
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD3	4	0.23	0.12	0.21
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	4	0.23	0.11	0.22
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	4	0.23	0.11	0.22
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	4	0.23	0.11	0.22
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	4	0.23	0.11	0.22
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	4	0.23	0.11	0.22
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	4	0.23	0.11	0.22
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG21	4	0.22	0.01	0.22
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG22	4	0.22	0.01	0.22
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG23	4	0.22	0.01	0.22
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG21	4	0.22	0.01	0.22
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG22	4	0.22	0.01	0.22
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG23	4	0.22	0.01	0.22
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG12	4	0.2	0.02	0.2
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG13	4	0.2	0.02	0.2
(1,878)	1:92:A:ALA:HA	1:95:A:GLU:HB2	4	0.2	0.02	0.2
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE1	4	0.19	0.07	0.18
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE2	4	0.19	0.07	0.18
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE3	4	0.19	0.07	0.18
(1,579)	1:132:A:THR:HB	1:133:A:GLY:H	4	0.19	0.02	0.18
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE1	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE2	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE3	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE1	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE2	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE3	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE1	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE2	4	0.19	0.04	0.19
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE3	4	0.19	0.04	0.19
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD11	4	0.18	0.06	0.18
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD12	4	0.18	0.06	0.18
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD13	4	0.18	0.06	0.18
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD21	4	0.18	0.06	0.18
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD22	4	0.18	0.06	0.18
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD23	4	0.18	0.06	0.18
(1,640)	1:44:A:LYS:HB2	1:48:A:ASN:H	4	0.18	0.04	0.18
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG21	4	0.16	0.03	0.16
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG22	4	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)
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG23	4	0.16	0.03	0.16
(1,180)	1:58:A:ALA:HB1	1:62:A:THR:HB	4	0.16	0.06	0.14
(1,180)	1:58:A:ALA:HB2	1:62:A:THR:HB	4	0.16	0.06	0.14
(1,180)	1:58:A:ALA:HB3	1:62:A:THR:HB	4	0.16	0.06	0.14
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD11	4	0.15	0.07	0.12
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD12	4	0.15	0.07	0.12
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD13	4	0.15	0.07	0.12
(1,950)	1:116:A:MET:HE1	1:117:A:ILE:H	4	0.15	0.04	0.14
(1,950)	1:116:A:MET:HE2	1:117:A:ILE:H	4	0.15	0.04	0.14
(1,950)	1:116:A:MET:HE3	1:117:A:ILE:H	4	0.15	0.04	0.14
(1,1239)	1:88:A:ARG:HD2	1:89:A:PHE:H	4	0.14	0.04	0.12
(1,1239)	1:88:A:ARG:HD3	1:89:A:PHE:H	4	0.14	0.04	0.12
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE1	4	0.14	0.03	0.13
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE2	4	0.14	0.03	0.13
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD11	4	0.14	0.03	0.14
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD12	4	0.14	0.03	0.14
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD13	4	0.14	0.03	0.14
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD11	4	0.14	0.03	0.14
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD12	4	0.14	0.03	0.14
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD13	4	0.14	0.03	0.14
(1,1400)	1:128:A:ILE:HG12	1:129:A:GLN:H	4	0.14	0.01	0.14
(1,1400)	1:128:A:ILE:HG13	1:129:A:GLN:H	4	0.14	0.01	0.14
(1,886)	1:64:A:THR:HG21	1:67:A:LYS:HB3	4	0.13	0.02	0.14
(1,886)	1:64:A:THR:HG22	1:67:A:LYS:HB3	4	0.13	0.02	0.14
(1,886)	1:64:A:THR:HG23	1:67:A:LYS:HB3	4	0.13	0.02	0.14
(1,625)	1:140:A:GLN:HB3	1:142:A:THR:H	4	0.12	0.01	0.12
(1,750)	1:24:A:THR:H	1:24:A:THR:HG21	4	0.11	0.0	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG22	4	0.11	0.0	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG23	4	0.11	0.0	0.11
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	3	0.36	0.09	0.37
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	3	0.36	0.09	0.37
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	3	0.36	0.09	0.37
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD11	3	0.33	0.13	0.32
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD12	3	0.33	0.13	0.32
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD13	3	0.33	0.13	0.32
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG11	3	0.29	0.03	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG12	3	0.29	0.03	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG13	3	0.29	0.03	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG21	3	0.29	0.03	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG22	3	0.29	0.03	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG23	3	0.29	0.03	0.28
(1,537)	1:68:A:ILE:HA	1:70:A:GLU:H	3	0.29	0.09	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1237)	1:88:A:ARG:HG2	1:92:A:ALA:HA	3	0.28	0.12	0.32
(1,1237)	1:88:A:ARG:HG3	1:92:A:ALA:HA	3	0.28	0.12	0.32
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB2	3	0.28	0.13	0.33
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB3	3	0.28	0.13	0.33
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB2	3	0.28	0.13	0.33
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB3	3	0.28	0.13	0.33
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB2	3	0.28	0.13	0.33
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB3	3	0.28	0.13	0.33
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG11	3	0.28	0.07	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG12	3	0.28	0.07	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG13	3	0.28	0.07	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG21	3	0.28	0.07	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG22	3	0.28	0.07	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG23	3	0.28	0.07	0.32
(1,1321)	1:105:A:SER:HB2	1:106:A:SER:H	3	0.25	0.07	0.25
(1,1321)	1:105:A:SER:HB3	1:106:A:SER:H	3	0.25	0.07	0.25
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG21	3	0.24	0.13	0.15
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG22	3	0.24	0.13	0.15
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG23	3	0.24	0.13	0.15
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD2	3	0.24	0.06	0.27
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD3	3	0.24	0.06	0.27
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD1	3	0.23	0.07	0.18
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD2	3	0.23	0.07	0.18
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD1	3	0.23	0.07	0.18
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD2	3	0.23	0.07	0.18
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD1	3	0.23	0.07	0.18
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD2	3	0.23	0.07	0.18
(1,1498)	1:173:A:LYS:HG2	1:174:A:ASN:H	3	0.23	0.05	0.25
(1,1498)	1:173:A:LYS:HG3	1:174:A:ASN:H	3	0.23	0.05	0.25
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD11	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD12	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD13	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD21	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD22	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD23	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD11	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD12	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD13	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD21	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD22	3	0.2	0.04	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD23	3	0.2	0.04	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE1	3	0.2	0.0	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE2	3	0.2	0.0	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE3	3	0.2	0.0	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE1	3	0.2	0.0	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE2	3	0.2	0.0	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE3	3	0.2	0.0	0.2
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	3	0.19	0.04	0.19
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	3	0.19	0.04	0.19
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	3	0.19	0.04	0.19
(1,1428)	1:136:A:LYS:HE2	1:137:A:GLU:HA	3	0.19	0.05	0.19
(1,1428)	1:136:A:LYS:HE3	1:137:A:GLU:HA	3	0.19	0.05	0.19
(1,1371)	1:123:A:LEU:HD11	1:124:A:GLU:HA	3	0.19	0.02	0.18
(1,1371)	1:123:A:LEU:HD12	1:124:A:GLU:HA	3	0.19	0.02	0.18
(1,1371)	1:123:A:LEU:HD13	1:124:A:GLU:HA	3	0.19	0.02	0.18
(1,1371)	1:123:A:LEU:HD21	1:124:A:GLU:HA	3	0.19	0.02	0.18
(1,1371)	1:123:A:LEU:HD22	1:124:A:GLU:HA	3	0.19	0.02	0.18
(1,1371)	1:123:A:LEU:HD23	1:124:A:GLU:HA	3	0.19	0.02	0.18
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG2	3	0.18	0.01	0.18
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG3	3	0.18	0.01	0.18
(1,1347)	1:115:A:LEU:HD11	1:119:A:VAL:HB	3	0.18	0.06	0.16
(1,1347)	1:115:A:LEU:HD12	1:119:A:VAL:HB	3	0.18	0.06	0.16
(1,1347)	1:115:A:LEU:HD13	1:119:A:VAL:HB	3	0.18	0.06	0.16
(1,1347)	1:115:A:LEU:HD21	1:119:A:VAL:HB	3	0.18	0.06	0.16
(1,1347)	1:115:A:LEU:HD22	1:119:A:VAL:HB	3	0.18	0.06	0.16
(1,1347)	1:115:A:LEU:HD23	1:119:A:VAL:HB	3	0.18	0.06	0.16
(1,29)	1:102:A:LYS:H	1:102:A:LYS:HG3	3	0.18	0.05	0.19
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB2	3	0.18	0.03	0.19
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB3	3	0.18	0.03	0.19
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG21	3	0.15	0.03	0.14
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG22	3	0.15	0.03	0.14
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG23	3	0.15	0.03	0.14
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG21	3	0.15	0.02	0.15
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG22	3	0.15	0.02	0.15
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG23	3	0.15	0.02	0.15
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB2	3	0.14	0.03	0.13
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB3	3	0.14	0.03	0.13
(1,556)	1:24:A:THR:HB	1:25:A:GLY:H	3	0.14	0.02	0.13
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB2	3	0.14	0.02	0.13
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB3	3	0.14	0.02	0.13
(1,455)	1:59:A:PHE:H	1:61:A:ASN:H	3	0.14	0.03	0.12
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB1	3	0.14	0.04	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB2	3	0.14	0.04	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB3	3	0.14	0.04	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB1	3	0.14	0.04	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB2	3	0.14	0.04	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB3	3	0.14	0.04	0.11
(1,840)	1:113:A:TYR:HE1	1:135:A:VAL:HA	3	0.13	0.01	0.13
(1,840)	1:113:A:TYR:HE2	1:135:A:VAL:HA	3	0.13	0.01	0.13
(1,203)	1:140:A:GLN:HA	1:140:A:GLN:HG3	3	0.12	0.01	0.13
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG21	3	0.12	0.02	0.11
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG22	3	0.12	0.02	0.11
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG23	3	0.12	0.02	0.11
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE1	3	0.12	0.02	0.11
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE2	3	0.12	0.02	0.11
(1,60)	1:91:A:LYS:HA	1:93:A:ILE:H	3	0.11	0.01	0.11
(1,979)	1:89:A:PHE:HE1	1:128:A:ILE:HB	3	0.11	0.01	0.1
(1,979)	1:89:A:PHE:HE2	1:128:A:ILE:HB	3	0.11	0.01	0.1
(1,830)	1:80:A:ILE:HD11	1:169:A:HIS:HE1	3	0.11	0.01	0.11
(1,830)	1:80:A:ILE:HD12	1:169:A:HIS:HE1	3	0.11	0.01	0.11
(1,830)	1:80:A:ILE:HD13	1:169:A:HIS:HE1	3	0.11	0.01	0.11
(1,1317)	1:102:A:LYS:HG2	1:103:A:SER:HA	2	1.12	0.13	1.12
(1,1317)	1:102:A:LYS:HG3	1:103:A:SER:HA	2	1.12	0.13	1.12
(1,281)	1:50:A:LYS:HA	1:50:A:LYS:HD3	2	0.4	0.05	0.4
(1,1162)	1:69:A:SER:HB2	1:70:A:GLU:HG2	2	0.36	0.0	0.36
(1,1162)	1:69:A:SER:HB2	1:70:A:GLU:HG3	2	0.36	0.0	0.36
(1,1162)	1:69:A:SER:HB3	1:70:A:GLU:HG2	2	0.36	0.0	0.36
(1,1162)	1:69:A:SER:HB3	1:70:A:GLU:HG3	2	0.36	0.0	0.36
(1,134)	1:140:A:GLN:H	1:140:A:GLN:HG2	2	0.34	0.16	0.34
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG11	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG12	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG13	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG21	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG22	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG23	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG11	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG12	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG13	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG21	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG22	2	0.34	0.12	0.34
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG23	2	0.34	0.12	0.34
(1,28)	1:102:A:LYS:H	1:102:A:LYS:HG2	2	0.33	0.01	0.33
(1,1096)	1:50:A:LYS:HA	1:50:A:LYS:HD2	2	0.33	0.02	0.33
(1,1096)	1:50:A:LYS:HA	1:50:A:LYS:HD3	2	0.33	0.02	0.33
(1,606)	1:70:A:GLU:H	1:70:A:GLU:HG3	2	0.32	0.08	0.32
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD11	2	0.32	0.12	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD12	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD13	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD21	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD22	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD23	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD11	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD12	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD13	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD21	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD22	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD23	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD11	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD12	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD13	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD21	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD22	2	0.32	0.12	0.32
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD23	2	0.32	0.12	0.32
(1,135)	1:140:A:GLN:H	1:140:A:GLN:HG3	2	0.3	0.2	0.3
(1,1303)	1:101:A:LYS:HB2	1:102:A:LYS:H	2	0.3	0.01	0.3
(1,1303)	1:101:A:LYS:HB3	1:102:A:LYS:H	2	0.3	0.01	0.3
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG21	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG22	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG23	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG21	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG22	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG23	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG21	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG22	2	0.29	0.11	0.29
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG23	2	0.29	0.11	0.29
(1,439)	1:102:A:LYS:H	1:103:A:SER:H	2	0.29	0.0	0.29
(1,1164)	1:70:A:GLU:H	1:70:A:GLU:HG2	2	0.28	0.02	0.28
(1,1164)	1:70:A:GLU:H	1:70:A:GLU:HG3	2	0.28	0.02	0.28
(1,800)	1:83:A:ILE:HD11	1:169:A:HIS:H	2	0.25	0.02	0.25
(1,800)	1:83:A:ILE:HD12	1:169:A:HIS:H	2	0.25	0.02	0.25
(1,800)	1:83:A:ILE:HD13	1:169:A:HIS:H	2	0.25	0.02	0.25
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB1	2	0.25	0.04	0.25
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB2	2	0.25	0.04	0.25
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB3	2	0.25	0.04	0.25
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB1	2	0.25	0.04	0.25
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB2	2	0.25	0.04	0.25
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB3	2	0.25	0.04	0.25
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD11	2	0.24	0.03	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD12	2	0.24	0.03	0.24
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD13	2	0.24	0.03	0.24
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD11	2	0.24	0.03	0.24
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD12	2	0.24	0.03	0.24
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD13	2	0.24	0.03	0.24
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD11	2	0.23	0.11	0.23
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD12	2	0.23	0.11	0.23
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD13	2	0.23	0.11	0.23
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG11	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG12	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG13	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG21	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG22	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG23	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG11	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG12	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG13	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG21	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG22	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG23	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG11	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG12	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG13	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG21	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG22	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG23	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG11	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG12	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG13	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG21	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG22	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG23	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG11	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG12	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG13	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG21	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG22	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG23	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG11	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG12	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG13	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG21	2	0.23	0.01	0.23

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG22	2	0.23	0.01	0.23
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG23	2	0.23	0.01	0.23
(1,1143)	1:63:A:GLN:H	1:63:A:GLN:HG2	2	0.22	0.07	0.22
(1,1143)	1:63:A:GLN:H	1:63:A:GLN:HG3	2	0.22	0.07	0.22
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB1	2	0.21	0.06	0.21
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB2	2	0.21	0.06	0.21
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB3	2	0.21	0.06	0.21
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD11	2	0.21	0.05	0.21
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD12	2	0.21	0.05	0.21
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD13	2	0.21	0.05	0.21
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD11	2	0.21	0.05	0.21
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD12	2	0.21	0.05	0.21
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD13	2	0.21	0.05	0.21
(1,598)	1:61:A:ASN:HB2	1:63:A:GLN:H	2	0.2	0.03	0.2
(1,1116)	1:54:A:VAL:HG11	1:59:A:PHE:HE1	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG11	1:59:A:PHE:HE2	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG12	1:59:A:PHE:HE1	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG12	1:59:A:PHE:HE2	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG13	1:59:A:PHE:HE1	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG13	1:59:A:PHE:HE2	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG21	1:59:A:PHE:HE1	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG21	1:59:A:PHE:HE2	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG22	1:59:A:PHE:HE1	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG22	1:59:A:PHE:HE2	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG23	1:59:A:PHE:HE1	2	0.2	0.0	0.2
(1,1116)	1:54:A:VAL:HG23	1:59:A:PHE:HE2	2	0.2	0.0	0.2
(1,1511)	1:177:A:GLU:HA	1:177:A:GLU:HG2	2	0.19	0.07	0.19
(1,1511)	1:177:A:GLU:HA	1:177:A:GLU:HG3	2	0.19	0.07	0.19
(1,193)	1:85:A:VAL:HA	1:88:A:ARG:HA	2	0.18	0.06	0.18
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE1	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE2	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE3	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE1	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE2	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE3	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE1	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE2	2	0.18	0.04	0.18
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE3	2	0.18	0.04	0.18
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE1	2	0.18	0.06	0.18
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE2	2	0.18	0.06	0.18
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE3	2	0.18	0.06	0.18
(1,189)	1:83:A:ILE:HD11	1:168:A:GLN:HA	2	0.17	0.03	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,189)	1:83:A:ILE:HD12	1:168:A:GLN:HA	2	0.17	0.03	0.17
(1,189)	1:83:A:ILE:HD13	1:168:A:GLN:HA	2	0.17	0.03	0.17
(1,288)	1:115:A:LEU:HB3	1:119:A:VAL:HB	2	0.16	0.02	0.16
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD11	2	0.16	0.02	0.16
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD12	2	0.16	0.02	0.16
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD13	2	0.16	0.02	0.16
(1,168)	1:151:A:ILE:HB	1:152:A:ALA:HA	2	0.16	0.02	0.16
(1,1495)	1:173:A:LYS:HA	1:173:A:LYS:HE2	2	0.16	0.02	0.16
(1,1495)	1:173:A:LYS:HA	1:173:A:LYS:HE3	2	0.16	0.02	0.16
(1,204)	1:97:A:ALA:HA	1:100:A:LEU:HG	2	0.16	0.01	0.16
(1,730)	1:90:A:VAL:HG11	1:160:A:LYS:H	2	0.16	0.05	0.16
(1,730)	1:90:A:VAL:HG12	1:160:A:LYS:H	2	0.16	0.05	0.16
(1,730)	1:90:A:VAL:HG13	1:160:A:LYS:H	2	0.16	0.05	0.16
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG21	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG22	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG23	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG21	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG22	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG23	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG21	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG22	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG23	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG21	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG22	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG23	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG21	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG22	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG23	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG21	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG22	2	0.16	0.01	0.16
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG23	2	0.16	0.01	0.16
(1,1022)	1:27:A:THR:H	1:28:A:LYS:HB2	2	0.15	0.0	0.15
(1,1022)	1:27:A:THR:H	1:28:A:LYS:HB3	2	0.15	0.0	0.15
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG11	2	0.15	0.03	0.15
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG12	2	0.15	0.03	0.15
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG13	2	0.15	0.03	0.15
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG21	2	0.15	0.03	0.15
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG22	2	0.15	0.03	0.15
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG23	2	0.15	0.03	0.15
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB1	2	0.15	0.03	0.15
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB2	2	0.15	0.03	0.15
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB3	2	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)
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB1	2	0.15	0.03	0.15
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB2	2	0.15	0.03	0.15
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB3	2	0.15	0.03	0.15
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG21	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG22	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG23	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG21	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG22	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG23	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG21	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG22	2	0.14	0.03	0.14
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG23	2	0.14	0.03	0.14
(1,238)	1:56:A:PHE:HA	1:59:A:PHE:HB3	2	0.14	0.02	0.14
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG21	2	0.14	0.02	0.14
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG22	2	0.14	0.02	0.14
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG23	2	0.14	0.02	0.14
(1,1031)	1:28:A:LYS:HB2	1:29:A:ILE:HG12	2	0.14	0.01	0.14
(1,1031)	1:28:A:LYS:HB2	1:29:A:ILE:HG13	2	0.14	0.01	0.14
(1,1031)	1:28:A:LYS:HB3	1:29:A:ILE:HG12	2	0.14	0.01	0.14
(1,1031)	1:28:A:LYS:HB3	1:29:A:ILE:HG13	2	0.14	0.01	0.14
(1,31)	1:131:A:MET:HE1	1:161:A:LEU:H	2	0.14	0.02	0.14
(1,31)	1:131:A:MET:HE2	1:161:A:LEU:H	2	0.14	0.02	0.14
(1,31)	1:131:A:MET:HE3	1:161:A:LEU:H	2	0.14	0.02	0.14
(1,571)	1:158:A:GLU:HA	1:162:A:ASN:H	2	0.14	0.02	0.14
(1,715)	1:53:A:GLY:H	1:54:A:VAL:HB	2	0.14	0.01	0.14
(1,1023)	1:27:A:THR:H	1:28:A:LYS:HG2	2	0.14	0.04	0.14
(1,1023)	1:27:A:THR:H	1:28:A:LYS:HG3	2	0.14	0.04	0.14
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD11	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD12	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD13	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD11	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD12	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD13	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD11	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD12	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD13	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD11	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD12	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD13	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD11	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD12	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD13	2	0.14	0.02	0.14

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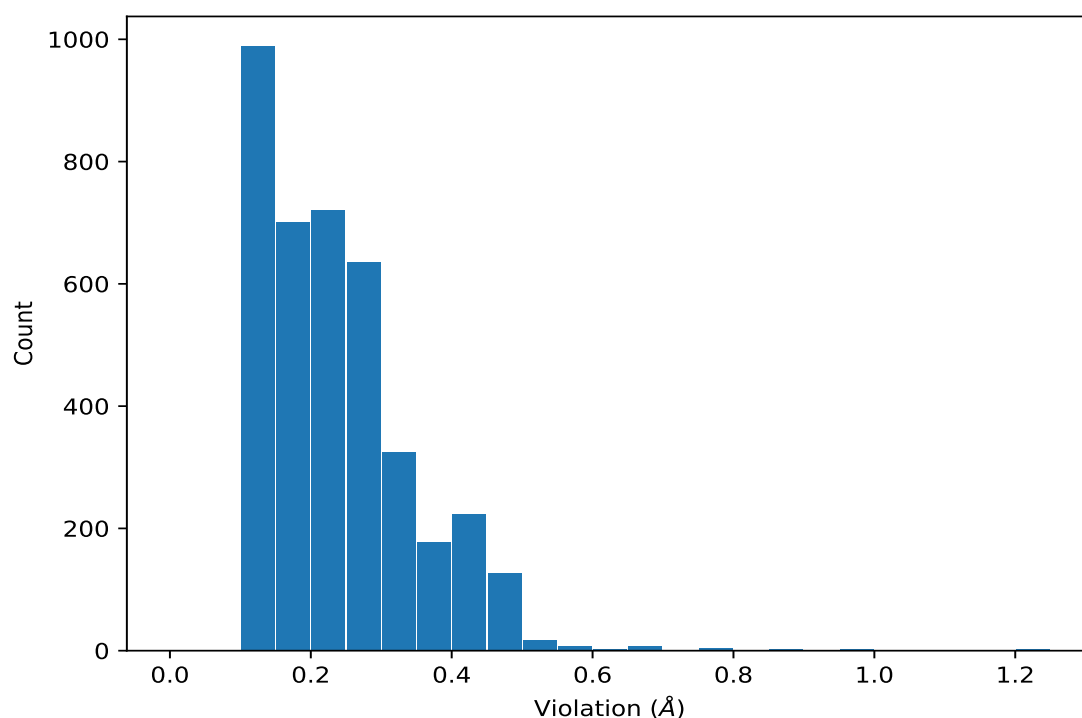
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD11	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD12	2	0.14	0.02	0.14
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD13	2	0.14	0.02	0.14
(1,1004)	1:45:A:ILE:HD11	1:74:A:PHE:HD1	2	0.13	0.03	0.13
(1,1004)	1:45:A:ILE:HD11	1:74:A:PHE:HD2	2	0.13	0.03	0.13
(1,1004)	1:45:A:ILE:HD12	1:74:A:PHE:HD1	2	0.13	0.03	0.13
(1,1004)	1:45:A:ILE:HD12	1:74:A:PHE:HD2	2	0.13	0.03	0.13
(1,1004)	1:45:A:ILE:HD13	1:74:A:PHE:HD1	2	0.13	0.03	0.13
(1,1004)	1:45:A:ILE:HD13	1:74:A:PHE:HD2	2	0.13	0.03	0.13
(1,1515)	1:177:A:GLU:HG2	1:179:A:ALA:H	2	0.13	0.03	0.13
(1,1515)	1:177:A:GLU:HG3	1:179:A:ALA:H	2	0.13	0.03	0.13
(1,530)	1:61:A:ASN:HA	1:62:A:THR:H	2	0.12	0.02	0.12
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE1	2	0.12	0.01	0.12
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE2	2	0.12	0.01	0.12
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE3	2	0.12	0.01	0.12
(1,1160)	1:68:A:ILE:HG12	1:69:A:SER:H	2	0.12	0.0	0.12
(1,1160)	1:68:A:ILE:HG13	1:69:A:SER:H	2	0.12	0.0	0.12
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG11	2	0.12	0.02	0.12
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG12	2	0.12	0.02	0.12
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG13	2	0.12	0.02	0.12
(1,440)	1:102:A:LYS:H	1:104:A:GLY:H	2	0.12	0.0	0.12
(1,597)	1:131:A:MET:HG2	1:132:A:THR:H	2	0.1	0.0	0.1

<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)
(1,1317)	1:102:A:LYS:HG2	1:103:A:SER:HA	9	1.25
(1,1317)	1:102:A:LYS:HG3	1:103:A:SER:HA	9	1.25
(1,1317)	1:102:A:LYS:HG2	1:103:A:SER:HA	10	0.99
(1,1317)	1:102:A:LYS:HG3	1:103:A:SER:HA	10	0.99
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	7	0.89
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	7	0.89
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB2	8	0.76
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB3	8	0.76
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB2	8	0.76
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB3	8	0.76
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	5	0.7
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	5	0.7
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	4	0.69
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	4	0.69
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	4	0.69
(1,1365)	1:122:A:PRO:HA	1:124:A:GLU:HG2	2	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1365)	1:122:A:PRO:HA	1:124:A:GLU:HG3	2	0.66
(1,1129)	1:56:A:PHE:HA	1:57:A:GLU:HG2	7	0.64
(1,1129)	1:56:A:PHE:HA	1:57:A:GLU:HG3	7	0.64
(1,535)	1:62:A:THR:HB	1:63:A:GLN:H	6	0.61
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	3	0.6
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	3	0.6
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	1	0.57
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	1	0.57
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	1	0.57
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	1	0.57
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	1	0.57
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	1	0.57
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	6	0.53
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	6	0.53
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	6	0.53
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	10	0.52
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	10	0.52
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB2	8	0.51
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB3	8	0.51
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB2	8	0.51
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB3	8	0.51
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB2	8	0.51
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB3	8	0.51
(1,200)	1:29:A:ILE:HB	1:30:A:ARG:HA	2	0.5
(1,135)	1:140:A:GLN:H	1:140:A:GLN:HG3	9	0.5
(1,134)	1:140:A:GLN:H	1:140:A:GLN:HG2	9	0.5
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD11	2	0.5
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD12	2	0.5
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD13	2	0.5
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	5	0.49
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	5	0.49
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	5	0.49
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	5	0.49
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	5	0.49
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	5	0.49
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	5	0.49
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	5	0.49
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	5	0.49
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	5	0.49
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	5	0.49
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	5	0.49
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG2	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG3	3	0.49
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG2	3	0.49
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG3	3	0.49
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG2	3	0.49
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG3	3	0.49
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	4	0.49
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	4	0.49
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	2	0.49
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	2	0.49
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	2	0.49
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	1	0.48
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	1	0.48
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	1	0.48
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	1	0.48
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	1	0.48
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	1	0.48
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	9	0.48
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	9	0.48
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	9	0.48
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	9	0.48
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	9	0.48
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	9	0.48
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG12	2	0.48
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG13	2	0.48
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	7	0.48
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	7	0.48
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	5	0.48
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	5	0.48
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	5	0.48
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	2	0.48
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	2	0.48
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	10	0.48
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	10	0.48
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	10	0.48
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	9	0.48
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	9	0.48
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	9	0.48
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	4	0.48
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	2	0.48
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	2	0.48
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	2	0.48
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	6	0.47
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	6	0.47
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	6	0.47
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	6	0.47
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	6	0.47
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	10	0.47
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	10	0.47
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	10	0.47
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE1	5	0.47
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE2	5	0.47
(1,535)	1:62:A:THR:HB	1:63:A:GLN:H	7	0.47
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG11	4	0.46
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG12	4	0.46
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG13	4	0.46
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG21	4	0.46
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG22	4	0.46
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG23	4	0.46
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG11	4	0.46
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG12	4	0.46
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG13	4	0.46
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG21	4	0.46
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG22	4	0.46
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG23	4	0.46
(1,1306)	1:101:A:LYS:HB2	1:147:A:ALA:HA	10	0.46
(1,1306)	1:101:A:LYS:HB3	1:147:A:ALA:HA	10	0.46
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG2	7	0.46
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG3	7	0.46
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG2	7	0.46
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG3	7	0.46
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG2	7	0.46
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG3	7	0.46
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	4	0.46
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	4	0.46
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	8	0.46
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	8	0.46
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	8	0.46
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	7	0.46
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	7	0.46
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	7	0.46
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	4	0.46
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	4	0.46
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	5	0.46
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	5	0.46
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	5	0.46
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	6	0.46
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	6	0.46
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	6	0.46
(1,1224)	1:86:A:ALA:HB1	1:87:A:GLU:HG2	2	0.45
(1,1224)	1:86:A:ALA:HB1	1:87:A:GLU:HG3	2	0.45
(1,1224)	1:86:A:ALA:HB2	1:87:A:GLU:HG2	2	0.45
(1,1224)	1:86:A:ALA:HB2	1:87:A:GLU:HG3	2	0.45
(1,1224)	1:86:A:ALA:HB3	1:87:A:GLU:HG2	2	0.45
(1,1224)	1:86:A:ALA:HB3	1:87:A:GLU:HG3	2	0.45
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB2	5	0.45
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB3	5	0.45
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB2	5	0.45
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB3	5	0.45
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB2	5	0.45
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB3	5	0.45
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	10	0.45
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	5	0.45
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	5	0.45
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	5	0.45
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	5	0.45
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	5	0.45
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	5	0.45
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	5	0.45
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	5	0.45
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	5	0.45
(1,281)	1:50:A:LYS:HA	1:50:A:LYS:HD3	3	0.45
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB2	10	0.44
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB3	10	0.44
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB2	10	0.44
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB3	10	0.44
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB2	10	0.44
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB3	10	0.44
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	8	0.44
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	8	0.44
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	4	0.44
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	6	0.44
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	6	0.44
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	6	0.44
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	8	0.44
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	8	0.44
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD11	9	0.43
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD12	9	0.43
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD13	9	0.43
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD21	9	0.43
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD22	9	0.43
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD23	9	0.43
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD11	9	0.43
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD12	9	0.43
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD13	9	0.43
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD21	9	0.43
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD22	9	0.43
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD23	9	0.43
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD11	9	0.43
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD12	9	0.43
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD13	9	0.43
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD21	9	0.43
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD22	9	0.43
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD23	9	0.43
(1,1104)	1:51:A:LYS:HD2	1:52:A:GLU:H	6	0.43
(1,1104)	1:51:A:LYS:HD3	1:52:A:GLU:H	6	0.43
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	1	0.43
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	1	0.43
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	1	0.43
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	6	0.43
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	6	0.43
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	6	0.43
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	4	0.43
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	4	0.43
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	4	0.43
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	8	0.43
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	8	0.43
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	8	0.43
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG21	1	0.43
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG22	1	0.43
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG23	1	0.43
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG21	1	0.43
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG22	1	0.43
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG23	1	0.43
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG21	1	0.43
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG22	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG23	1	0.43
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG21	3	0.43
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG22	3	0.43
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG23	3	0.43
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG21	3	0.43
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG22	3	0.43
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG23	3	0.43
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG21	3	0.43
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG22	3	0.43
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG23	3	0.43
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	3	0.43
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	3	0.43
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG21	8	0.43
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG22	8	0.43
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG23	8	0.43
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	10	0.42
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	10	0.42
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	10	0.42
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	10	0.42
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	10	0.42
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	10	0.42
(1,1219)	1:85:A:VAL:HG11	1:87:A:GLU:HG2	2	0.42
(1,1219)	1:85:A:VAL:HG11	1:87:A:GLU:HG3	2	0.42
(1,1219)	1:85:A:VAL:HG12	1:87:A:GLU:HG2	2	0.42
(1,1219)	1:85:A:VAL:HG12	1:87:A:GLU:HG3	2	0.42
(1,1219)	1:85:A:VAL:HG13	1:87:A:GLU:HG2	2	0.42
(1,1219)	1:85:A:VAL:HG13	1:87:A:GLU:HG3	2	0.42
(1,1219)	1:85:A:VAL:HG21	1:87:A:GLU:HG2	2	0.42
(1,1219)	1:85:A:VAL:HG21	1:87:A:GLU:HG3	2	0.42
(1,1219)	1:85:A:VAL:HG22	1:87:A:GLU:HG2	2	0.42
(1,1219)	1:85:A:VAL:HG22	1:87:A:GLU:HG3	2	0.42
(1,1219)	1:85:A:VAL:HG23	1:87:A:GLU:HG2	2	0.42
(1,1219)	1:85:A:VAL:HG23	1:87:A:GLU:HG3	2	0.42
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB2	3	0.42
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB3	3	0.42
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB2	3	0.42
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB3	3	0.42
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	9	0.42
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	9	0.42
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	10	0.42
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	10	0.42
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	6	0.42
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	1	0.42
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	5	0.42
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG21	7	0.42
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG22	7	0.42
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG23	7	0.42
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE2	10	0.41
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE3	10	0.41
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE2	10	0.41
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE3	10	0.41
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE2	10	0.41
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE3	10	0.41
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE2	10	0.41
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE3	10	0.41
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE2	10	0.41
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE3	10	0.41
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE2	10	0.41
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE3	10	0.41
(1,1237)	1:88:A:ARG:HG2	1:92:A:ALA:HA	9	0.41
(1,1237)	1:88:A:ARG:HG3	1:92:A:ALA:HA	9	0.41
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG12	1	0.41
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG13	1	0.41
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	2	0.41
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	2	0.41
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	2	0.41
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	6	0.41
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	6	0.41
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	10	0.41
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	10	0.41
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	10	0.41
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	2	0.41
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	8	0.41
(1,535)	1:62:A:THR:HB	1:63:A:GLN:H	2	0.41
(1,535)	1:62:A:THR:HB	1:63:A:GLN:H	4	0.41
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	7	0.41
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	7	0.41
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	7	0.41
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG21	10	0.41
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG22	10	0.41
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG23	10	0.41
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	5	0.4
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	5	0.4
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	5	0.4
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	5	0.4
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	5	0.4
(1,1168)	1:72:A:PRO:HB2	1:175:A:LEU:HD11	4	0.4
(1,1168)	1:72:A:PRO:HB2	1:175:A:LEU:HD12	4	0.4
(1,1168)	1:72:A:PRO:HB2	1:175:A:LEU:HD13	4	0.4
(1,1168)	1:72:A:PRO:HB2	1:175:A:LEU:HD21	4	0.4
(1,1168)	1:72:A:PRO:HB2	1:175:A:LEU:HD22	4	0.4
(1,1168)	1:72:A:PRO:HB2	1:175:A:LEU:HD23	4	0.4
(1,1168)	1:72:A:PRO:HB3	1:175:A:LEU:HD11	4	0.4
(1,1168)	1:72:A:PRO:HB3	1:175:A:LEU:HD12	4	0.4
(1,1168)	1:72:A:PRO:HB3	1:175:A:LEU:HD13	4	0.4
(1,1168)	1:72:A:PRO:HB3	1:175:A:LEU:HD21	4	0.4
(1,1168)	1:72:A:PRO:HB3	1:175:A:LEU:HD22	4	0.4
(1,1168)	1:72:A:PRO:HB3	1:175:A:LEU:HD23	4	0.4
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG12	4	0.4
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG13	4	0.4
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB2	1	0.4
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB3	1	0.4
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB2	1	0.4
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB3	1	0.4
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB2	1	0.4
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB3	1	0.4
(1,1104)	1:51:A:LYS:HD2	1:52:A:GLU:H	3	0.4
(1,1104)	1:51:A:LYS:HD3	1:52:A:GLU:H	3	0.4
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB2	5	0.4
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB3	5	0.4
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB2	5	0.4
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB3	5	0.4
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB2	5	0.4
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB3	5	0.4
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	10	0.4
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG21	6	0.4
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG22	6	0.4
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG23	6	0.4
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG21	6	0.4
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG22	6	0.4
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG23	6	0.4
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG21	6	0.4
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG22	6	0.4
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG23	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD11	10	0.4
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD12	10	0.4
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD13	10	0.4
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	6	0.4
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	6	0.4
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	6	0.4
(1,606)	1:70:A:GLU:H	1:70:A:GLU:HG3	5	0.4
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	4	0.4
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	6	0.4
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	7	0.4
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	1	0.4
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	1	0.4
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	1	0.4
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	1	0.4
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	1	0.4
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	1	0.4
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	1	0.4
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	1	0.4
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	1	0.4
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	2	0.4
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	2	0.4
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	2	0.4
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	2	0.4
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	2	0.4
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	2	0.4
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	2	0.4
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	2	0.4
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	2	0.4
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	1	0.4
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	1	0.4
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	1	0.4
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	3	0.4
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	3	0.4
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	3	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	8	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	8	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	8	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	10	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	10	0.4
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	10	0.4
(1,122)	1:83:A:ILE:HD11	1:85:A:VAL:H	7	0.4
(1,122)	1:83:A:ILE:HD12	1:85:A:VAL:H	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:83:A:ILE:HD13	1:85:A:VAL:H	7	0.4
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD2	3	0.39
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD3	3	0.39
(1,1311)	1:101:A:LYS:HD2	1:103:A:SER:H	8	0.39
(1,1311)	1:101:A:LYS:HD3	1:103:A:SER:H	8	0.39
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	10	0.39
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	10	0.39
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	10	0.39
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	10	0.39
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	10	0.39
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	10	0.39
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	10	0.39
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	10	0.39
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	10	0.39
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	10	0.39
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	10	0.39
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	10	0.39
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	10	0.39
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	10	0.39
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	10	0.39
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	10	0.39
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	10	0.39
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	10	0.39
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD2	1	0.39
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD3	1	0.39
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	8	0.39
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	8	0.39
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	8	0.39
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	8	0.39
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	8	0.39
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	8	0.39
(1,1104)	1:51:A:LYS:HD2	1:52:A:GLU:H	7	0.39
(1,1104)	1:51:A:LYS:HD3	1:52:A:GLU:H	7	0.39
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG21	5	0.39
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG22	5	0.39
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG23	5	0.39
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG21	5	0.39
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG22	5	0.39
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG23	5	0.39
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG21	5	0.39
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG22	5	0.39
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG23	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	1	0.39
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	4	0.38
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	4	0.38
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	4	0.38
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	4	0.38
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	4	0.38
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	4	0.38
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG2	9	0.38
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG3	9	0.38
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG2	9	0.38
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG3	9	0.38
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG2	9	0.38
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG3	9	0.38
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	2	0.38
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	2	0.38
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	2	0.38
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	2	0.38
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	2	0.38
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	2	0.38
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	5	0.38
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	1	0.38
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	8	0.38
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	8	0.38
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	8	0.38
(1,108)	1:129:A:GLN:H	1:132:A:THR:HG21	2	0.38
(1,108)	1:129:A:GLN:H	1:132:A:THR:HG22	2	0.38
(1,108)	1:129:A:GLN:H	1:132:A:THR:HG23	2	0.38
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	10	0.37
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	10	0.37
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	6	0.37
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	6	0.37
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	6	0.37
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	6	0.37
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	6	0.37
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	6	0.37
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	10	0.37
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	10	0.37
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	10	0.37
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	10	0.37
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	10	0.37
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	10	0.37
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG2	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG3	5	0.37
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG2	5	0.37
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG3	5	0.37
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG2	5	0.37
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG3	5	0.37
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD1	1	0.37
(1,990)	1:52:A:GLU:HA	1:56:A:PHE:HD2	1	0.37
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	4	0.37
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	8	0.37
(1,794)	1:68:A:ILE:HD11	1:69:A:SER:H	1	0.37
(1,794)	1:68:A:ILE:HD12	1:69:A:SER:H	1	0.37
(1,794)	1:68:A:ILE:HD13	1:69:A:SER:H	1	0.37
(1,794)	1:68:A:ILE:HD11	1:69:A:SER:H	9	0.37
(1,794)	1:68:A:ILE:HD12	1:69:A:SER:H	9	0.37
(1,794)	1:68:A:ILE:HD13	1:69:A:SER:H	9	0.37
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD11	1	0.37
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD12	1	0.37
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD13	1	0.37
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	10	0.37
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	10	0.37
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	10	0.37
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	6	0.37
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	6	0.37
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	2	0.37
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	6	0.37
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	7	0.37
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	9	0.37
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	7	0.37
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	7	0.37
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	7	0.37
(1,207)	1:90:A:VAL:HG21	1:154:A:ALA:HA	1	0.37
(1,207)	1:90:A:VAL:HG22	1:154:A:ALA:HA	1	0.37
(1,207)	1:90:A:VAL:HG23	1:154:A:ALA:HA	1	0.37
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	1	0.37
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	2	0.36
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	2	0.36
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	2	0.36
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	2	0.36
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	2	0.36
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	2	0.36
(1,1405)	1:129:A:GLN:HG2	1:130:A:LYS:HE2	8	0.36
(1,1405)	1:129:A:GLN:HG2	1:130:A:LYS:HE3	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1405)	1:129:A:GLN:HG3	1:130:A:LYS:HE2	8	0.36
(1,1405)	1:129:A:GLN:HG3	1:130:A:LYS:HE3	8	0.36
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	7	0.36
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	7	0.36
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	7	0.36
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	7	0.36
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	7	0.36
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	7	0.36
(1,1162)	1:69:A:SER:HB2	1:70:A:GLU:HG2	2	0.36
(1,1162)	1:69:A:SER:HB2	1:70:A:GLU:HG3	2	0.36
(1,1162)	1:69:A:SER:HB3	1:70:A:GLU:HG2	2	0.36
(1,1162)	1:69:A:SER:HB3	1:70:A:GLU:HG3	2	0.36
(1,1162)	1:69:A:SER:HB2	1:70:A:GLU:HG2	3	0.36
(1,1162)	1:69:A:SER:HB2	1:70:A:GLU:HG3	3	0.36
(1,1162)	1:69:A:SER:HB3	1:70:A:GLU:HG2	3	0.36
(1,1162)	1:69:A:SER:HB3	1:70:A:GLU:HG3	3	0.36
(1,1104)	1:51:A:LYS:HD2	1:52:A:GLU:H	2	0.36
(1,1104)	1:51:A:LYS:HD3	1:52:A:GLU:H	2	0.36
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	3	0.36
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	3	0.36
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	3	0.36
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	3	0.36
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	3	0.36
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	3	0.36
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	3	0.36
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	8	0.36
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	8	0.36
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	8	0.36
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD11	5	0.36
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD12	5	0.36
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD13	5	0.36
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	2	0.36
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	2	0.36
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	2	0.36
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	3	0.36
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	10	0.36
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	8	0.36
(1,537)	1:68:A:ILE:HA	1:70:A:GLU:H	3	0.36
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	3	0.36
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	3	0.36
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	3	0.36
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	3	0.36
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	3	0.36
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	3	0.36
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	3	0.36
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	3	0.36
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	3	0.36
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	3	0.36
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	3	0.36
(1,122)	1:83:A:ILE:HD11	1:85:A:VAL:H	5	0.36
(1,122)	1:83:A:ILE:HD12	1:85:A:VAL:H	5	0.36
(1,122)	1:83:A:ILE:HD13	1:85:A:VAL:H	5	0.36
(1,1311)	1:101:A:LYS:HD2	1:103:A:SER:H	2	0.35
(1,1311)	1:101:A:LYS:HD3	1:103:A:SER:H	2	0.35
(1,1306)	1:101:A:LYS:HB2	1:147:A:ALA:HA	8	0.35
(1,1306)	1:101:A:LYS:HB3	1:147:A:ALA:HA	8	0.35
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD2	9	0.35
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD3	9	0.35
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	9	0.35
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	9	0.35
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	9	0.35
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	9	0.35
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	9	0.35
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	9	0.35
(1,1096)	1:50:A:LYS:HA	1:50:A:LYS:HD2	6	0.35
(1,1096)	1:50:A:LYS:HA	1:50:A:LYS:HD3	6	0.35
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	3	0.35
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	3	0.35
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	3	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	3	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	3	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	3	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	6	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	6	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	6	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	9	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	9	0.35
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	9	0.35
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG21	8	0.35
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG22	8	0.35
(1,914)	1:100:A:LEU:HD21	1:146:A:THR:HG23	8	0.35
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG21	8	0.35
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG22	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:100:A:LEU:HD22	1:146:A:THR:HG23	8	0.35
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG21	8	0.35
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG22	8	0.35
(1,914)	1:100:A:LEU:HD23	1:146:A:THR:HG23	8	0.35
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	7	0.35
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	9	0.35
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	1	0.35
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	4	0.35
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	7	0.35
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	6	0.35
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	6	0.35
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	6	0.35
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	6	0.35
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	6	0.35
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	6	0.35
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	6	0.35
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	6	0.35
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	6	0.35
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	4	0.35
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	4	0.35
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	4	0.35
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	10	0.35
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	10	0.35
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	10	0.35
(1,281)	1:50:A:LYS:HA	1:50:A:LYS:HD3	6	0.35
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG21	1	0.35
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG22	1	0.35
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG23	1	0.35
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	8	0.34
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	8	0.34
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	8	0.34
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	8	0.34
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	8	0.34
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	8	0.34
(1,1321)	1:105:A:SER:HB2	1:106:A:SER:H	6	0.34
(1,1321)	1:105:A:SER:HB3	1:106:A:SER:H	6	0.34
(1,1311)	1:101:A:LYS:HD2	1:103:A:SER:H	7	0.34
(1,1311)	1:101:A:LYS:HD3	1:103:A:SER:H	7	0.34
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	4	0.34
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	4	0.34
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	4	0.34
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	4	0.34
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	4	0.34
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE1	1	0.34
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE2	1	0.34
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE3	1	0.34
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE1	1	0.34
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE2	1	0.34
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE3	1	0.34
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	4	0.34
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	4	0.34
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	4	0.34
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	4	0.34
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	4	0.34
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	4	0.34
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	7	0.34
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	7	0.34
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	7	0.34
(1,794)	1:68:A:ILE:HD11	1:69:A:SER:H	6	0.34
(1,794)	1:68:A:ILE:HD12	1:69:A:SER:H	6	0.34
(1,794)	1:68:A:ILE:HD13	1:69:A:SER:H	6	0.34
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	3	0.34
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	3	0.34
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	3	0.34
(1,537)	1:68:A:ILE:HA	1:70:A:GLU:H	7	0.34
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	8	0.34
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	9	0.34
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD11	1	0.34
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD12	1	0.34
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD13	1	0.34
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG21	6	0.34
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG22	6	0.34
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG23	6	0.34
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	9	0.34
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	9	0.34
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	9	0.34
(1,207)	1:90:A:VAL:HG21	1:154:A:ALA:HA	3	0.34
(1,207)	1:90:A:VAL:HG22	1:154:A:ALA:HA	3	0.34
(1,207)	1:90:A:VAL:HG23	1:154:A:ALA:HA	3	0.34
(1,28)	1:102:A:LYS:H	1:102:A:LYS:HG2	2	0.34
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG11	9	0.33
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG12	9	0.33
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG13	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG21	9	0.33
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG22	9	0.33
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG23	9	0.33
(1,1312)	1:101:A:LYS:HE2	1:147:A:ALA:HB1	2	0.33
(1,1312)	1:101:A:LYS:HE2	1:147:A:ALA:HB2	2	0.33
(1,1312)	1:101:A:LYS:HE2	1:147:A:ALA:HB3	2	0.33
(1,1312)	1:101:A:LYS:HE3	1:147:A:ALA:HB1	2	0.33
(1,1312)	1:101:A:LYS:HE3	1:147:A:ALA:HB2	2	0.33
(1,1312)	1:101:A:LYS:HE3	1:147:A:ALA:HB3	2	0.33
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE1	6	0.33
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE2	6	0.33
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE3	6	0.33
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE1	6	0.33
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE2	6	0.33
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE3	6	0.33
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG11	7	0.33
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG12	7	0.33
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG13	7	0.33
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG21	7	0.33
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG22	7	0.33
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG23	7	0.33
(1,1081)	1:46:A:LYS:HD2	1:47:A:ALA:H	7	0.33
(1,1081)	1:46:A:LYS:HD3	1:47:A:ALA:H	7	0.33
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB2	8	0.33
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB3	8	0.33
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB2	8	0.33
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB3	8	0.33
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB2	8	0.33
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB3	8	0.33
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	5	0.33
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	5	0.33
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	5	0.33
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	9	0.33
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	9	0.33
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	9	0.33
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	2	0.33
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	9	0.33
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD1	7	0.33
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD2	7	0.33
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD1	7	0.33
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD2	7	0.33
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD1	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD2	7	0.33
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	1	0.33
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	1	0.33
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	1	0.33
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD11	9	0.33
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD12	9	0.33
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD13	9	0.33
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	6	0.33
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	6	0.33
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	6	0.33
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	1	0.33
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	8	0.33
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	5	0.33
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	7	0.33
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	4	0.33
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	4	0.33
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	4	0.33
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	4	0.33
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	4	0.33
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	4	0.33
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	4	0.33
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	4	0.33
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	4	0.33
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG21	7	0.33
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG22	7	0.33
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG23	7	0.33
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	8	0.33
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	8	0.33
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	8	0.33
(1,68)	1:88:A:ARG:HD2	1:92:A:ALA:H	1	0.33
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG11	5	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG12	5	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG13	5	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG21	5	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG22	5	0.32
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG23	5	0.32
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	6	0.32
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	6	0.32
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	6	0.32
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	6	0.32
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	6	0.32
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	9	0.32
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	9	0.32
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	9	0.32
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	9	0.32
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	9	0.32
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	9	0.32
(1,1237)	1:88:A:ARG:HG2	1:92:A:ALA:HA	8	0.32
(1,1237)	1:88:A:ARG:HG3	1:92:A:ALA:HA	8	0.32
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	7	0.32
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	7	0.32
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	7	0.32
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	7	0.32
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	7	0.32
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	7	0.32
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	7	0.32
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	7	0.32
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	7	0.32
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	7	0.32
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	7	0.32
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	7	0.32
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	7	0.32
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	7	0.32
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	7	0.32
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	7	0.32
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	7	0.32
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	7	0.32
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	3	0.32
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	3	0.32
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	6	0.32
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	6	0.32
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	4	0.32
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	4	0.32
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	4	0.32
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	4	0.32
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	2	0.32
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	2	0.32
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	2	0.32
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	7	0.32
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	7	0.32
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	7	0.32
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	9	0.32
(1,393)	1:88:A:ARG:H	1:88:A:ARG:HG3	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG21	4	0.32
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG22	4	0.32
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG23	4	0.32
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	4	0.32
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	4	0.32
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	4	0.32
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	7	0.32
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	7	0.32
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	7	0.32
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG21	5	0.32
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG22	5	0.32
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG23	5	0.32
(1,122)	1:83:A:ILE:HD11	1:85:A:VAL:H	6	0.32
(1,122)	1:83:A:ILE:HD12	1:85:A:VAL:H	6	0.32
(1,122)	1:83:A:ILE:HD13	1:85:A:VAL:H	6	0.32
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD11	6	0.32
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD12	6	0.32
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD13	6	0.32
(1,28)	1:102:A:LYS:H	1:102:A:LYS:HG2	8	0.32
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE1	8	0.31
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE2	8	0.31
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE3	8	0.31
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE1	8	0.31
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE2	8	0.31
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE3	8	0.31
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	8	0.31
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	8	0.31
(1,1303)	1:101:A:LYS:HB2	1:102:A:LYS:H	10	0.31
(1,1303)	1:101:A:LYS:HB3	1:102:A:LYS:H	10	0.31
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	10	0.31
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	10	0.31
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	2	0.31
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	2	0.31
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	2	0.31
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	2	0.31
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	2	0.31
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	2	0.31
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB2	1	0.31
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB3	1	0.31
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB2	1	0.31
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB3	1	0.31
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	10	0.31
(1,1096)	1:50:A:LYS:HA	1:50:A:LYS:HD2	3	0.31
(1,1096)	1:50:A:LYS:HA	1:50:A:LYS:HD3	3	0.31
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	2	0.31
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	2	0.31
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	10	0.31
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	10	0.31
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	10	0.31
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	10	0.31
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	8	0.31
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	8	0.31
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	8	0.31
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	2	0.31
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	2	0.31
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	2	0.31
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	8	0.31
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	8	0.31
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	8	0.31
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	3	0.31
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	3	0.31
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	3	0.31
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	3	0.31
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	3	0.31
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	3	0.31
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	5	0.31
(1,710)	1:98:A:GLU:H	1:99:A:LYS:HD2	2	0.31
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	3	0.31
(1,554)	1:63:A:GLN:HA	1:64:A:THR:H	5	0.31
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	10	0.31
(1,394)	1:88:A:ARG:H	1:88:A:ARG:HG2	10	0.31
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG21	2	0.31
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG22	2	0.31
(1,314)	1:62:A:THR:HA	1:62:A:THR:HG23	2	0.31
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	5	0.31
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	5	0.31
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	5	0.31
(1,200)	1:29:A:ILE:HB	1:30:A:ARG:HA	6	0.31
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	9	0.31
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	9	0.31
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	9	0.31
(1,86)	1:44:A:LYS:H	1:44:A:LYS:HB3	7	0.31
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE2	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE3	2	0.3
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE2	2	0.3
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE3	2	0.3
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE2	2	0.3
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE3	2	0.3
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE2	2	0.3
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE3	2	0.3
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE2	2	0.3
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE3	2	0.3
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE2	2	0.3
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE3	2	0.3
(1,1304)	1:101:A:LYS:HB2	1:103:A:SER:H	4	0.3
(1,1304)	1:101:A:LYS:HB3	1:103:A:SER:H	4	0.3
(1,1303)	1:101:A:LYS:HB2	1:102:A:LYS:H	9	0.3
(1,1303)	1:101:A:LYS:HB3	1:102:A:LYS:H	9	0.3
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB1	1	0.3
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB2	1	0.3
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB3	1	0.3
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB1	1	0.3
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB2	1	0.3
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB3	1	0.3
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	2	0.3
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	2	0.3
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	2	0.3
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	2	0.3
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	2	0.3
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	2	0.3
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	5	0.3
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	5	0.3
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	5	0.3
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	5	0.3
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	5	0.3
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	5	0.3
(1,1188)	1:74:A:PHE:HZ	1:75:A:ILE:HG12	2	0.3
(1,1188)	1:74:A:PHE:HZ	1:75:A:ILE:HG13	2	0.3
(1,1164)	1:70:A:GLU:H	1:70:A:GLU:HG2	2	0.3
(1,1164)	1:70:A:GLU:H	1:70:A:GLU:HG3	2	0.3
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	8	0.3
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	8	0.3
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG12	4	0.3
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG13	4	0.3
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG12	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG13	4	0.3
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG12	4	0.3
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG13	4	0.3
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD11	3	0.3
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD12	3	0.3
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD13	3	0.3
(1,924)	1:45:A:ILE:HD11	1:46:A:LYS:HA	6	0.3
(1,924)	1:45:A:ILE:HD12	1:46:A:LYS:HA	6	0.3
(1,924)	1:45:A:ILE:HD13	1:46:A:LYS:HA	6	0.3
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	7	0.3
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	7	0.3
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	7	0.3
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD11	6	0.3
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD12	6	0.3
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD13	6	0.3
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	4	0.3
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	4	0.3
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	4	0.3
(1,765)	1:150:A:ILE:HG21	1:153:A:ILE:H	6	0.3
(1,765)	1:150:A:ILE:HG22	1:153:A:ILE:H	6	0.3
(1,765)	1:150:A:ILE:HG23	1:153:A:ILE:H	6	0.3
(1,709)	1:98:A:GLU:H	1:99:A:LYS:HD3	5	0.3
(1,709)	1:98:A:GLU:H	1:99:A:LYS:HD3	6	0.3
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	10	0.3
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	2	0.3
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	10	0.3
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	1	0.3
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	2	0.3
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	4	0.3
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	7	0.3
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	10	0.3
(1,363)	1:134:A:THR:HG21	1:138:A:ALA:HB1	6	0.3
(1,363)	1:134:A:THR:HG21	1:138:A:ALA:HB2	6	0.3
(1,363)	1:134:A:THR:HG21	1:138:A:ALA:HB3	6	0.3
(1,363)	1:134:A:THR:HG22	1:138:A:ALA:HB1	6	0.3
(1,363)	1:134:A:THR:HG22	1:138:A:ALA:HB2	6	0.3
(1,363)	1:134:A:THR:HG22	1:138:A:ALA:HB3	6	0.3
(1,363)	1:134:A:THR:HG23	1:138:A:ALA:HB1	6	0.3
(1,363)	1:134:A:THR:HG23	1:138:A:ALA:HB2	6	0.3
(1,363)	1:134:A:THR:HG23	1:138:A:ALA:HB3	6	0.3
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE1	8	0.3
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE2	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE3	8	0.3
(1,69)	1:88:A:ARG:HD3	1:92:A:ALA:H	7	0.3
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD2	7	0.29
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD3	7	0.29
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB1	7	0.29
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB2	7	0.29
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB3	7	0.29
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB1	7	0.29
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB2	7	0.29
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB3	7	0.29
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD2	1	0.29
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD3	1	0.29
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	7	0.29
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	7	0.29
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	2	0.29
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	2	0.29
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	2	0.29
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	2	0.29
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	2	0.29
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	2	0.29
(1,1169)	1:72:A:PRO:HG2	1:175:A:LEU:HD11	4	0.29
(1,1169)	1:72:A:PRO:HG2	1:175:A:LEU:HD12	4	0.29
(1,1169)	1:72:A:PRO:HG2	1:175:A:LEU:HD13	4	0.29
(1,1169)	1:72:A:PRO:HG2	1:175:A:LEU:HD21	4	0.29
(1,1169)	1:72:A:PRO:HG2	1:175:A:LEU:HD22	4	0.29
(1,1169)	1:72:A:PRO:HG2	1:175:A:LEU:HD23	4	0.29
(1,1169)	1:72:A:PRO:HG3	1:175:A:LEU:HD11	4	0.29
(1,1169)	1:72:A:PRO:HG3	1:175:A:LEU:HD12	4	0.29
(1,1169)	1:72:A:PRO:HG3	1:175:A:LEU:HD13	4	0.29
(1,1169)	1:72:A:PRO:HG3	1:175:A:LEU:HD21	4	0.29
(1,1169)	1:72:A:PRO:HG3	1:175:A:LEU:HD22	4	0.29
(1,1169)	1:72:A:PRO:HG3	1:175:A:LEU:HD23	4	0.29
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	6	0.29
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	6	0.29
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	6	0.29
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	6	0.29
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	6	0.29
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	6	0.29
(1,1151)	1:66:A:SER:HB2	1:67:A:LYS:HB3	8	0.29
(1,1151)	1:66:A:SER:HB3	1:67:A:LYS:HB3	8	0.29
(1,1143)	1:63:A:GLN:H	1:63:A:GLN:HG2	7	0.29
(1,1143)	1:63:A:GLN:H	1:63:A:GLN:HG3	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG12	7	0.29
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG13	7	0.29
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG11	7	0.29
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG12	7	0.29
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG13	7	0.29
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG21	7	0.29
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG22	7	0.29
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG23	7	0.29
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	6	0.29
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	6	0.29
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	6	0.29
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	6	0.29
(1,1000)	1:42:A:ILE:HA	1:44:A:LYS:HB2	6	0.29
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	6	0.29
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	8	0.29
(1,765)	1:150:A:ILE:HG21	1:153:A:ILE:H	2	0.29
(1,765)	1:150:A:ILE:HG22	1:153:A:ILE:H	2	0.29
(1,765)	1:150:A:ILE:HG23	1:153:A:ILE:H	2	0.29
(1,709)	1:98:A:GLU:H	1:99:A:LYS:HD3	4	0.29
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	4	0.29
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	4	0.29
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	6	0.29
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	8	0.29
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	3	0.29
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	9	0.29
(1,439)	1:102:A:LYS:H	1:103:A:SER:H	7	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	3	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	3	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	3	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	9	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	9	0.29
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	9	0.29
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	2	0.29
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	2	0.29
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	2	0.29
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	6	0.29
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	6	0.29
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	6	0.29
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	7	0.29
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	7	0.29
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE2	7	0.28
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE3	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE2	7	0.28
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE3	7	0.28
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE2	7	0.28
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE3	7	0.28
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE2	7	0.28
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE3	7	0.28
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE2	7	0.28
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE3	7	0.28
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE2	7	0.28
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE3	7	0.28
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	4	0.28
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	4	0.28
(1,1306)	1:101:A:LYS:HB2	1:147:A:ALA:HA	9	0.28
(1,1306)	1:101:A:LYS:HB3	1:147:A:ALA:HA	9	0.28
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB1	3	0.28
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB2	3	0.28
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB3	3	0.28
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB1	3	0.28
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB2	3	0.28
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB3	3	0.28
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	2	0.28
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	2	0.28
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	2	0.28
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	2	0.28
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	2	0.28
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	2	0.28
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	4	0.28
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	4	0.28
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	4	0.28
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	4	0.28
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	4	0.28
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	4	0.28
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	5	0.28
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	5	0.28
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	5	0.28
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	5	0.28
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	5	0.28
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	5	0.28
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	5	0.28
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	5	0.28
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	5	0.28
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	5	0.28
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	5	0.28
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	5	0.28
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	5	0.28
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	5	0.28
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	5	0.28
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	5	0.28
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	5	0.28
(1,1148)	1:64:A:THR:HG21	1:67:A:LYS:HE2	2	0.28
(1,1148)	1:64:A:THR:HG21	1:67:A:LYS:HE3	2	0.28
(1,1148)	1:64:A:THR:HG22	1:67:A:LYS:HE2	2	0.28
(1,1148)	1:64:A:THR:HG22	1:67:A:LYS:HE3	2	0.28
(1,1148)	1:64:A:THR:HG23	1:67:A:LYS:HE2	2	0.28
(1,1148)	1:64:A:THR:HG23	1:67:A:LYS:HE3	2	0.28
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB2	3	0.28
(1,1138)	1:62:A:THR:HG21	1:63:A:GLN:HB3	3	0.28
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB2	3	0.28
(1,1138)	1:62:A:THR:HG22	1:63:A:GLN:HB3	3	0.28
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB2	3	0.28
(1,1138)	1:62:A:THR:HG23	1:63:A:GLN:HB3	3	0.28
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	3	0.28
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	3	0.28
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	4	0.28
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	4	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG11	3	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG12	3	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG13	3	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG21	3	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG22	3	0.28
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG23	3	0.28
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	1	0.28
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	1	0.28
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	1	0.28
(1,976)	1:56:A:PHE:HA	1:56:A:PHE:HZ	1	0.28
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD11	1	0.28
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD12	1	0.28
(1,969)	1:146:A:THR:H	1:153:A:ILE:HD13	1	0.28
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	8	0.28
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	10	0.28
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	10	0.28
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	10	0.28
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	10	0.28
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	10	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	1	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	1	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	1	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	7	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	7	0.28
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	7	0.28
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	4	0.28
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	4	0.28
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	5	0.28
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	5	0.28
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	7	0.28
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	7	0.28
(1,657)	1:122:A:PRO:HG3	1:123:A:LEU:H	6	0.28
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	4	0.28
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	2	0.28
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	5	0.28
(1,439)	1:102:A:LYS:H	1:103:A:SER:H	3	0.28
(1,394)	1:88:A:ARG:H	1:88:A:ARG:HG2	3	0.28
(1,394)	1:88:A:ARG:H	1:88:A:ARG:HG2	7	0.28
(1,393)	1:88:A:ARG:H	1:88:A:ARG:HG3	6	0.28
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG21	5	0.28
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG22	5	0.28
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG23	5	0.28
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	10	0.28
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	10	0.28
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	10	0.28
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	3	0.28
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	3	0.28
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	3	0.28
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	8	0.28
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	8	0.28
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	8	0.28
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	10	0.28
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	10	0.28
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	10	0.28
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	2	0.28
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	2	0.28
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	2	0.28
(1,1498)	1:173:A:LYS:HG2	1:174:A:ASN:H	8	0.27
(1,1498)	1:173:A:LYS:HG3	1:174:A:ASN:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	7	0.27
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	7	0.27
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	9	0.27
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	9	0.27
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD2	2	0.27
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD3	2	0.27
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD11	9	0.27
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD12	9	0.27
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD13	9	0.27
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD11	9	0.27
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD12	9	0.27
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD13	9	0.27
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD11	4	0.27
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD12	4	0.27
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD13	4	0.27
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD21	4	0.27
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD22	4	0.27
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD23	4	0.27
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB2	10	0.27
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB3	10	0.27
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB2	10	0.27
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB3	10	0.27
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE2	5	0.27
(1,1059)	1:39:A:LYS:H	1:39:A:LYS:HE3	5	0.27
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	2	0.27
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	2	0.27
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	2	0.27
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	2	0.27
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	3	0.27
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	3	0.27
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	3	0.27
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG21	5	0.27
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG22	5	0.27
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG23	5	0.27
(1,800)	1:83:A:ILE:HD11	1:169:A:HIS:H	9	0.27
(1,800)	1:83:A:ILE:HD12	1:169:A:HIS:H	9	0.27
(1,800)	1:83:A:ILE:HD13	1:169:A:HIS:H	9	0.27
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	1	0.27
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	1	0.27
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	1	0.27
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	9	0.27
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	9	0.27
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD11	10	0.27
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD12	10	0.27
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD13	10	0.27
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB1	3	0.27
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB2	3	0.27
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB3	3	0.27
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	7	0.27
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	7	0.27
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	7	0.27
(1,710)	1:98:A:GLU:H	1:99:A:LYS:HD2	8	0.27
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	8	0.27
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	8	0.27
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	10	0.27
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	10	0.27
(1,587)	1:72:A:PRO:HD3	1:73:A:GLU:H	4	0.27
(1,538)	1:67:A:LYS:HA	1:68:A:ILE:H	3	0.27
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	2	0.27
(1,393)	1:88:A:ARG:H	1:88:A:ARG:HG3	2	0.27
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	10	0.27
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	10	0.27
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	10	0.27
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	10	0.27
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	10	0.27
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	10	0.27
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	10	0.27
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	10	0.27
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	10	0.27
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	5	0.27
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	5	0.27
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	5	0.27
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	9	0.27
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	9	0.27
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	9	0.27
(1,200)	1:29:A:ILE:HB	1:30:A:ARG:HA	5	0.27
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	10	0.27
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	10	0.27
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	10	0.27
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	8	0.27
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	8	0.27
(1,1511)	1:177:A:GLU:HA	1:177:A:GLU:HG2	8	0.26
(1,1511)	1:177:A:GLU:HA	1:177:A:GLU:HG3	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	10	0.26
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	10	0.26
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	10	0.26
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	10	0.26
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	10	0.26
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	10	0.26
(1,1347)	1:115:A:LEU:HD11	1:119:A:VAL:HB	6	0.26
(1,1347)	1:115:A:LEU:HD12	1:119:A:VAL:HB	6	0.26
(1,1347)	1:115:A:LEU:HD13	1:119:A:VAL:HB	6	0.26
(1,1347)	1:115:A:LEU:HD21	1:119:A:VAL:HB	6	0.26
(1,1347)	1:115:A:LEU:HD22	1:119:A:VAL:HB	6	0.26
(1,1347)	1:115:A:LEU:HD23	1:119:A:VAL:HB	6	0.26
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB2	7	0.26
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB3	7	0.26
(1,1318)	1:102:A:LYS:HG2	1:103:A:SER:HB2	10	0.26
(1,1318)	1:102:A:LYS:HG2	1:103:A:SER:HB3	10	0.26
(1,1318)	1:102:A:LYS:HG3	1:103:A:SER:HB2	10	0.26
(1,1318)	1:102:A:LYS:HG3	1:103:A:SER:HB3	10	0.26
(1,1311)	1:101:A:LYS:HD2	1:103:A:SER:H	1	0.26
(1,1311)	1:101:A:LYS:HD3	1:103:A:SER:H	1	0.26
(1,1306)	1:101:A:LYS:HB2	1:147:A:ALA:HA	3	0.26
(1,1306)	1:101:A:LYS:HB3	1:147:A:ALA:HA	3	0.26
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	10	0.26
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	10	0.26
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	10	0.26
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	10	0.26
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	10	0.26
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	10	0.26
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	2	0.26
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	2	0.26
(1,1255)	1:95:A:GLU:H	1:95:A:GLU:HG2	6	0.26
(1,1255)	1:95:A:GLU:H	1:95:A:GLU:HG3	6	0.26
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB2	8	0.26
(1,1249)	1:92:A:ALA:HB1	1:95:A:GLU:HB3	8	0.26
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB2	8	0.26
(1,1249)	1:92:A:ALA:HB2	1:95:A:GLU:HB3	8	0.26
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB2	8	0.26
(1,1249)	1:92:A:ALA:HB3	1:95:A:GLU:HB3	8	0.26
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	3	0.26
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	3	0.26
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	3	0.26
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	3	0.26
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	3	0.26
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB2	9	0.26
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB3	9	0.26
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB2	9	0.26
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB3	9	0.26
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	2	0.26
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	2	0.26
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG11	1	0.26
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG12	1	0.26
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG13	1	0.26
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG21	1	0.26
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG22	1	0.26
(1,1089)	1:49:A:ALA:HA	1:54:A:VAL:HG23	1	0.26
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG12	10	0.26
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG13	10	0.26
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG12	10	0.26
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG13	10	0.26
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG12	10	0.26
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG13	10	0.26
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD11	1	0.26
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD12	1	0.26
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD13	1	0.26
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD11	1	0.26
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD12	1	0.26
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD13	1	0.26
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	5	0.26
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	5	0.26
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	5	0.26
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	5	0.26
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	5	0.26
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	5	0.26
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	5	0.26
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	5	0.26
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	5	0.26
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD21	7	0.26
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD22	7	0.26
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD23	7	0.26
(1,710)	1:98:A:GLU:H	1:99:A:LYS:HD2	3	0.26
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	9	0.26
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	6	0.26
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:88:A:ARG:H	1:88:A:ARG:HG2	1	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	7	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	7	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	7	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	7	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	7	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	7	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	7	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	7	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	7	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	8	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	8	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	8	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	8	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	8	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	8	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	8	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	8	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	8	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG21	9	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG22	9	0.26
(1,368)	1:150:A:ILE:HD11	1:153:A:ILE:HG23	9	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG21	9	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG22	9	0.26
(1,368)	1:150:A:ILE:HD12	1:153:A:ILE:HG23	9	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG21	9	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG22	9	0.26
(1,368)	1:150:A:ILE:HD13	1:153:A:ILE:HG23	9	0.26
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	4	0.26
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	4	0.26
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	4	0.26
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	3	0.26
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	9	0.26
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	6	0.26
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	6	0.26
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	9	0.26
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	9	0.26
(1,69)	1:88:A:ARG:HD3	1:92:A:ALA:H	10	0.26
(1,1498)	1:173:A:LYS:HG2	1:174:A:ASN:H	2	0.25
(1,1498)	1:173:A:LYS:HG3	1:174:A:ASN:H	2	0.25
(1,1481)	1:170:A:ASP:HA	1:173:A:LYS:HB2	6	0.25
(1,1481)	1:170:A:ASP:HA	1:173:A:LYS:HB3	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG12	8	0.25
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG13	8	0.25
(1,1428)	1:136:A:LYS:HE2	1:137:A:GLU:HA	3	0.25
(1,1428)	1:136:A:LYS:HE3	1:137:A:GLU:HA	3	0.25
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	6	0.25
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	6	0.25
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	6	0.25
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	6	0.25
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	6	0.25
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	6	0.25
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	6	0.25
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	6	0.25
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	6	0.25
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	6	0.25
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	6	0.25
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	6	0.25
(1,1321)	1:105:A:SER:HB2	1:106:A:SER:H	8	0.25
(1,1321)	1:105:A:SER:HB3	1:106:A:SER:H	8	0.25
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	8	0.25
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	8	0.25
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	8	0.25
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	8	0.25
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	8	0.25
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	8	0.25
(1,1248)	1:92:A:ALA:HA	1:95:A:GLU:HG2	6	0.25
(1,1248)	1:92:A:ALA:HA	1:95:A:GLU:HG3	6	0.25
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD11	7	0.25
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD12	7	0.25
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD13	7	0.25
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD21	7	0.25
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD22	7	0.25
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD23	7	0.25
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD11	7	0.25
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD12	7	0.25
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD13	7	0.25
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD21	7	0.25
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD22	7	0.25
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD23	7	0.25
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	4	0.25
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	4	0.25
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	4	0.25
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	4	0.25
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	4	0.25
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	10	0.25
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	10	0.25
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	10	0.25
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	10	0.25
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	10	0.25
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	10	0.25
(1,1164)	1:70:A:GLU:H	1:70:A:GLU:HG2	5	0.25
(1,1164)	1:70:A:GLU:H	1:70:A:GLU:HG3	5	0.25
(1,1082)	1:47:A:ALA:HA	1:50:A:LYS:HB2	6	0.25
(1,1082)	1:47:A:ALA:HA	1:50:A:LYS:HB3	6	0.25
(1,1078)	1:46:A:LYS:HA	1:46:A:LYS:HD2	1	0.25
(1,1078)	1:46:A:LYS:HA	1:46:A:LYS:HD3	1	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	5	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	5	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	5	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	5	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	5	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	5	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	9	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	9	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	9	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	9	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	9	0.25
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	9	0.25
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	1	0.25
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	1	0.25
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	1	0.25
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	1	0.25
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	3	0.25
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	3	0.25
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	3	0.25
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD1	2	0.25
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD2	2	0.25
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD1	7	0.25
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD2	7	0.25
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE1	4	0.25
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE2	4	0.25
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	7	0.25
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	7	0.25
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	7	0.25
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	7	0.25
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	7	0.25
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	10	0.25
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	10	0.25
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	10	0.25
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	2	0.25
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	2	0.25
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	2	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD11	3	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD12	3	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD13	3	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD11	10	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD12	10	0.25
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD13	10	0.25
(1,710)	1:98:A:GLU:H	1:99:A:LYS:HD2	7	0.25
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	3	0.25
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	3	0.25
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	7	0.25
(1,606)	1:70:A:GLU:H	1:70:A:GLU:HG3	2	0.25
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	9	0.25
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	3	0.25
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	10	0.25
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	10	0.25
(1,357)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	10	0.25
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	1	0.25
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	1	0.25
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	1	0.25
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	9	0.25
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	9	0.25
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	9	0.25
(1,233)	1:80:A:ILE:HD11	1:81:A:LYS:HA	8	0.25
(1,233)	1:80:A:ILE:HD12	1:81:A:LYS:HA	8	0.25
(1,233)	1:80:A:ILE:HD13	1:81:A:LYS:HA	8	0.25
(1,180)	1:58:A:ALA:HB1	1:62:A:THR:HB	8	0.25
(1,180)	1:58:A:ALA:HB2	1:62:A:THR:HB	8	0.25
(1,180)	1:58:A:ALA:HB3	1:62:A:THR:HB	8	0.25
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	7	0.25
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	7	0.25
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	7	0.25
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	2	0.25
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	3	0.25
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	3	0.25
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	4	0.25
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	4	0.25
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG11	5	0.24
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG12	5	0.24
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG13	5	0.24
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG21	5	0.24
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG22	5	0.24
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG23	5	0.24
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG11	5	0.24
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG12	5	0.24
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG13	5	0.24
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG21	5	0.24
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG22	5	0.24
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG23	5	0.24
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG11	5	0.24
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG12	5	0.24
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG13	5	0.24
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG21	5	0.24
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG22	5	0.24
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG23	5	0.24
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG11	5	0.24
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG12	5	0.24
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG13	5	0.24
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG21	5	0.24
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG22	5	0.24
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG23	5	0.24
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG11	5	0.24
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG12	5	0.24
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG13	5	0.24
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG21	5	0.24
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG22	5	0.24
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG23	5	0.24
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG11	5	0.24
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG12	5	0.24
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG13	5	0.24
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG21	5	0.24
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG22	5	0.24
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG23	5	0.24
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG12	1	0.24
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG13	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	4	0.24
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	4	0.24
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	4	0.24
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	4	0.24
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	4	0.24
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	4	0.24
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	1	0.24
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	1	0.24
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	8	0.24
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	8	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG11	1	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG12	1	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG13	1	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG21	1	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG22	1	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG23	1	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG11	5	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG12	5	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG13	5	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG21	5	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG22	5	0.24
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG23	5	0.24
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	4	0.24
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	4	0.24
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	4	0.24
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	4	0.24
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	4	0.24
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	4	0.24
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	3	0.24
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	6	0.24
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE1	7	0.24
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE2	7	0.24
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE3	7	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	5	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	5	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	5	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	8	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	8	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	8	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	9	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	9	0.24
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD11	4	0.24
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD12	4	0.24
(1,796)	1:27:A:THR:H	1:29:A:ILE:HD13	4	0.24
(1,794)	1:68:A:ILE:HD11	1:69:A:SER:H	10	0.24
(1,794)	1:68:A:ILE:HD12	1:69:A:SER:H	10	0.24
(1,794)	1:68:A:ILE:HD13	1:69:A:SER:H	10	0.24
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	10	0.24
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	10	0.24
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	10	0.24
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD21	4	0.24
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD22	4	0.24
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD23	4	0.24
(1,710)	1:98:A:GLU:H	1:99:A:LYS:HD2	10	0.24
(1,640)	1:44:A:LYS:HB2	1:48:A:ASN:H	8	0.24
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	10	0.24
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	6	0.24
(1,598)	1:61:A:ASN:HB2	1:63:A:GLN:H	6	0.24
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	5	0.24
(1,393)	1:88:A:ARG:H	1:88:A:ARG:HG3	9	0.24
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG21	9	0.24
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG22	9	0.24
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG23	9	0.24
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	2	0.24
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	2	0.24
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	2	0.24
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE1	8	0.24
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE2	8	0.24
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE3	8	0.24
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE1	8	0.24
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE2	8	0.24
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE3	8	0.24
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE1	8	0.24
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE2	8	0.24
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE3	8	0.24
(1,271)	1:152:A:ALA:HB1	1:153:A:ILE:HA	5	0.24
(1,271)	1:152:A:ALA:HB2	1:153:A:ILE:HA	5	0.24
(1,271)	1:152:A:ALA:HB3	1:153:A:ILE:HA	5	0.24
(1,193)	1:85:A:VAL:HA	1:88:A:ARG:HA	6	0.24
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	6	0.24
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	6	0.24
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	6	0.24
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	10	0.24
(1,69)	1:88:A:ARG:HD3	1:92:A:ALA:H	3	0.24
(1,65)	1:179:A:ALA:HA	1:180:A:LYS:H	2	0.24
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE1	9	0.23
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE2	9	0.23
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE3	9	0.23
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE1	9	0.23
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE2	9	0.23
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE3	9	0.23
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG2	6	0.23
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG3	6	0.23
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG2	6	0.23
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG3	6	0.23
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG2	6	0.23
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG3	6	0.23
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG2	6	0.23
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG3	6	0.23
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG2	6	0.23
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG3	6	0.23
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG2	6	0.23
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG3	6	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	9	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	9	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	9	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	9	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	9	0.23
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	9	0.23
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	6	0.23
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	6	0.23
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	6	0.23
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	6	0.23
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	6	0.23
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	6	0.23
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG12	6	0.23
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG13	6	0.23
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG12	10	0.23
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG13	10	0.23
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	6	0.23
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	6	0.23
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB2	9	0.23
(1,1123)	1:55:A:LYS:HA	1:56:A:PHE:HB3	9	0.23
(1,1119)	1:54:A:VAL:HG11	1:74:A:PHE:HZ	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1119)	1:54:A:VAL:HG12	1:74:A:PHE:HZ	7	0.23
(1,1119)	1:54:A:VAL:HG13	1:74:A:PHE:HZ	7	0.23
(1,1119)	1:54:A:VAL:HG21	1:74:A:PHE:HZ	7	0.23
(1,1119)	1:54:A:VAL:HG22	1:74:A:PHE:HZ	7	0.23
(1,1119)	1:54:A:VAL:HG23	1:74:A:PHE:HZ	7	0.23
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG12	1	0.23
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG13	1	0.23
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG12	1	0.23
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG13	1	0.23
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG12	1	0.23
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG13	1	0.23
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	4	0.23
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	1	0.23
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	1	0.23
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	1	0.23
(1,878)	1:92:A:ALA:HA	1:95:A:GLU:HB2	9	0.23
(1,870)	1:27:A:THR:HG21	1:28:A:LYS:HE2	6	0.23
(1,870)	1:27:A:THR:HG22	1:28:A:LYS:HE2	6	0.23
(1,870)	1:27:A:THR:HG23	1:28:A:LYS:HE2	6	0.23
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	9	0.23
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	9	0.23
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	9	0.23
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	9	0.23
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	9	0.23
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	9	0.23
(1,800)	1:83:A:ILE:HD11	1:169:A:HIS:H	4	0.23
(1,800)	1:83:A:ILE:HD12	1:169:A:HIS:H	4	0.23
(1,800)	1:83:A:ILE:HD13	1:169:A:HIS:H	4	0.23
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	5	0.23
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	5	0.23
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	5	0.23
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	2	0.23
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	2	0.23
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	2	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD21	1	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD22	1	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD23	1	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD21	5	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD22	5	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD23	5	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD21	8	0.23
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD22	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD23	8	0.23
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	3	0.23
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	3	0.23
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	3	0.23
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	7	0.23
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	7	0.23
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	7	0.23
(1,709)	1:98:A:GLU:H	1:99:A:LYS:HD3	9	0.23
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	9	0.23
(1,579)	1:132:A:THR:HB	1:133:A:GLY:H	3	0.23
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	7	0.23
(1,563)	1:139:A:ALA:H	1:140:A:GLN:HA	9	0.23
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	3	0.23
(1,540)	1:115:A:LEU:HA	1:117:A:ILE:H	1	0.23
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	6	0.23
(1,207)	1:90:A:VAL:HG21	1:154:A:ALA:HA	2	0.23
(1,207)	1:90:A:VAL:HG22	1:154:A:ALA:HA	2	0.23
(1,207)	1:90:A:VAL:HG23	1:154:A:ALA:HA	2	0.23
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG21	8	0.23
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG22	8	0.23
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG23	8	0.23
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG21	8	0.23
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG22	8	0.23
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG23	8	0.23
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG21	9	0.23
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG22	9	0.23
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG23	9	0.23
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG21	9	0.23
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG22	9	0.23
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG23	9	0.23
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	3	0.23
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	3	0.23
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	3	0.23
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	1	0.23
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	1	0.23
(1,29)	1:102:A:LYS:H	1:102:A:LYS:HG3	8	0.23
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG11	9	0.22
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG12	9	0.22
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG13	9	0.22
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG21	9	0.22
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG22	9	0.22
(1,1461)	1:161:A:LEU:HD11	1:164:A:VAL:HG23	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG11	9	0.22
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG12	9	0.22
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG13	9	0.22
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG21	9	0.22
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG22	9	0.22
(1,1461)	1:161:A:LEU:HD12	1:164:A:VAL:HG23	9	0.22
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG11	9	0.22
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG12	9	0.22
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG13	9	0.22
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG21	9	0.22
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG22	9	0.22
(1,1461)	1:161:A:LEU:HD13	1:164:A:VAL:HG23	9	0.22
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG11	9	0.22
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG12	9	0.22
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG13	9	0.22
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG21	9	0.22
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG22	9	0.22
(1,1461)	1:161:A:LEU:HD21	1:164:A:VAL:HG23	9	0.22
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG11	9	0.22
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG12	9	0.22
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG13	9	0.22
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG21	9	0.22
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG22	9	0.22
(1,1461)	1:161:A:LEU:HD22	1:164:A:VAL:HG23	9	0.22
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG11	9	0.22
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG12	9	0.22
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG13	9	0.22
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG21	9	0.22
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG22	9	0.22
(1,1461)	1:161:A:LEU:HD23	1:164:A:VAL:HG23	9	0.22
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE1	9	0.22
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE2	9	0.22
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE3	9	0.22
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE1	9	0.22
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE2	9	0.22
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE3	9	0.22
(1,1371)	1:123:A:LEU:HD11	1:124:A:GLU:HA	6	0.22
(1,1371)	1:123:A:LEU:HD12	1:124:A:GLU:HA	6	0.22
(1,1371)	1:123:A:LEU:HD13	1:124:A:GLU:HA	6	0.22
(1,1371)	1:123:A:LEU:HD21	1:124:A:GLU:HA	6	0.22
(1,1371)	1:123:A:LEU:HD22	1:124:A:GLU:HA	6	0.22
(1,1371)	1:123:A:LEU:HD23	1:124:A:GLU:HA	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB2	4	0.22
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB3	4	0.22
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	7	0.22
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	7	0.22
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	7	0.22
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	7	0.22
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	7	0.22
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	7	0.22
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	9	0.22
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	9	0.22
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	9	0.22
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	9	0.22
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	9	0.22
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	9	0.22
(1,1239)	1:88:A:ARG:HD2	1:89:A:PHE:H	1	0.22
(1,1239)	1:88:A:ARG:HD3	1:89:A:PHE:H	1	0.22
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	9	0.22
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	9	0.22
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	9	0.22
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	9	0.22
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	9	0.22
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	9	0.22
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	9	0.22
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	9	0.22
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	9	0.22
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	9	0.22
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	9	0.22
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	9	0.22
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	9	0.22
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	9	0.22
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	9	0.22
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	9	0.22
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	9	0.22
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	9	0.22
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD11	4	0.22
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD12	4	0.22
(1,1205)	1:80:A:ILE:HG12	1:83:A:ILE:HD13	4	0.22
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD11	4	0.22
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD12	4	0.22
(1,1205)	1:80:A:ILE:HG13	1:83:A:ILE:HD13	4	0.22
(1,1104)	1:51:A:LYS:HD2	1:52:A:GLU:H	10	0.22
(1,1104)	1:51:A:LYS:HD3	1:52:A:GLU:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:80:A:ILE:HD11	1:84:A:GLN:H	7	0.22
(1,1002)	1:80:A:ILE:HD12	1:84:A:GLN:H	7	0.22
(1,1002)	1:80:A:ILE:HD13	1:84:A:GLN:H	7	0.22
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD11	1	0.22
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD12	1	0.22
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD13	1	0.22
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	5	0.22
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	7	0.22
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG21	4	0.22
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG22	4	0.22
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG23	4	0.22
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG21	7	0.22
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG22	7	0.22
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG23	7	0.22
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	2	0.22
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	2	0.22
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	2	0.22
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	8	0.22
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	8	0.22
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	8	0.22
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	9	0.22
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	9	0.22
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	8	0.22
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	6	0.22
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	8	0.22
(1,393)	1:88:A:ARG:H	1:88:A:ARG:HG3	4	0.22
(1,393)	1:88:A:ARG:H	1:88:A:ARG:HG3	8	0.22
(1,376)	1:72:A:PRO:HA	1:75:A:ILE:HD11	4	0.22
(1,376)	1:72:A:PRO:HA	1:75:A:ILE:HD12	4	0.22
(1,376)	1:72:A:PRO:HA	1:75:A:ILE:HD13	4	0.22
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE1	7	0.22
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE2	7	0.22
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE3	7	0.22
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE1	7	0.22
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE2	7	0.22
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE3	7	0.22
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE1	7	0.22
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE2	7	0.22
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE3	7	0.22
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE1	3	0.22
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE2	3	0.22
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE3	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE1	3	0.22
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE2	3	0.22
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE3	3	0.22
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE1	3	0.22
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE2	3	0.22
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE3	3	0.22
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG21	5	0.22
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG22	5	0.22
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG23	5	0.22
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG21	5	0.22
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG22	5	0.22
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG23	5	0.22
(1,112)	1:49:A:ALA:HB1	1:54:A:VAL:H	5	0.22
(1,112)	1:49:A:ALA:HB2	1:54:A:VAL:H	5	0.22
(1,112)	1:49:A:ALA:HB3	1:54:A:VAL:H	5	0.22
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	10	0.22
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	10	0.22
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	10	0.22
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	3	0.21
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	3	0.21
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG12	3	0.21
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG13	3	0.21
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG11	8	0.21
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG12	8	0.21
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG13	8	0.21
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG21	8	0.21
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG22	8	0.21
(1,1414)	1:130:A:LYS:HD2	1:164:A:VAL:HG23	8	0.21
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG11	8	0.21
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG12	8	0.21
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG13	8	0.21
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG21	8	0.21
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG22	8	0.21
(1,1414)	1:130:A:LYS:HD3	1:164:A:VAL:HG23	8	0.21
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE1	1	0.21
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE2	1	0.21
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE3	1	0.21
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE1	1	0.21
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE2	1	0.21
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE3	1	0.21
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB1	6	0.21
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB2	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:101:A:LYS:HG2	1:147:A:ALA:HB3	6	0.21
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB1	6	0.21
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB2	6	0.21
(1,1310)	1:101:A:LYS:HG3	1:147:A:ALA:HB3	6	0.21
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB1	8	0.21
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB2	8	0.21
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB3	8	0.21
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB1	8	0.21
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB2	8	0.21
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB3	8	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	4	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	4	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	4	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	4	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	4	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	4	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	7	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	7	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	7	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	7	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	7	0.21
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	7	0.21
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	4	0.21
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	4	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	8	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	8	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	8	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	8	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	8	0.21
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	8	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	8	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	8	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	8	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	8	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	8	0.21
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	8	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	8	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	8	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	8	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	8	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	8	0.21
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD11	5	0.21
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD12	5	0.21
(1,1179)	1:73:A:GLU:HB2	1:80:A:ILE:HD13	5	0.21
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD11	5	0.21
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD12	5	0.21
(1,1179)	1:73:A:GLU:HB3	1:80:A:ILE:HD13	5	0.21
(1,1116)	1:54:A:VAL:HG11	1:59:A:PHE:HE1	8	0.21
(1,1116)	1:54:A:VAL:HG11	1:59:A:PHE:HE2	8	0.21
(1,1116)	1:54:A:VAL:HG12	1:59:A:PHE:HE1	8	0.21
(1,1116)	1:54:A:VAL:HG12	1:59:A:PHE:HE2	8	0.21
(1,1116)	1:54:A:VAL:HG13	1:59:A:PHE:HE1	8	0.21
(1,1116)	1:54:A:VAL:HG13	1:59:A:PHE:HE2	8	0.21
(1,1116)	1:54:A:VAL:HG21	1:59:A:PHE:HE1	8	0.21
(1,1116)	1:54:A:VAL:HG21	1:59:A:PHE:HE2	8	0.21
(1,1116)	1:54:A:VAL:HG22	1:59:A:PHE:HE1	8	0.21
(1,1116)	1:54:A:VAL:HG22	1:59:A:PHE:HE2	8	0.21
(1,1116)	1:54:A:VAL:HG23	1:59:A:PHE:HE1	8	0.21
(1,1116)	1:54:A:VAL:HG23	1:59:A:PHE:HE2	8	0.21
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG11	3	0.21
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG12	3	0.21
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG13	3	0.21
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG21	3	0.21
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG22	3	0.21
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG23	3	0.21
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	2	0.21
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	2	0.21
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	2	0.21
(1,950)	1:116:A:MET:HE1	1:117:A:ILE:H	7	0.21
(1,950)	1:116:A:MET:HE2	1:117:A:ILE:H	7	0.21
(1,950)	1:116:A:MET:HE3	1:117:A:ILE:H	7	0.21
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	1	0.21
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	1	0.21
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	1	0.21
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	1	0.21
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	1	0.21
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	1	0.21
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	1	0.21
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	1	0.21
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	1	0.21
(1,825)	1:48:A:ASN:H	1:49:A:ALA:HA	6	0.21
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	4	0.21
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	4	0.21
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD11	7	0.21
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD12	7	0.21
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD13	7	0.21
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	7	0.21
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	7	0.21
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	2	0.21
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	4	0.21
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	2	0.21
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	9	0.21
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB1	1	0.21
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB2	1	0.21
(1,246)	1:113:A:TYR:HB3	1:144:A:ALA:HB3	1	0.21
(1,200)	1:29:A:ILE:HB	1:30:A:ARG:HA	1	0.21
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG21	6	0.21
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG22	6	0.21
(1,149)	1:89:A:PHE:HE1	1:126:A:ILE:HG23	6	0.21
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG21	6	0.21
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG22	6	0.21
(1,149)	1:89:A:PHE:HE2	1:126:A:ILE:HG23	6	0.21
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG21	1	0.21
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG22	1	0.21
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG23	1	0.21
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	4	0.21
(1,83)	1:52:A:GLU:H	1:52:A:GLU:HG2	3	0.21
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG12	6	0.2
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG13	6	0.2
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD11	5	0.2
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD12	5	0.2
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD13	5	0.2
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD21	5	0.2
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD22	5	0.2
(1,1420)	1:131:A:MET:HE1	1:161:A:LEU:HD23	5	0.2
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD11	5	0.2
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD12	5	0.2
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD13	5	0.2
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD21	5	0.2
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD22	5	0.2
(1,1420)	1:131:A:MET:HE2	1:161:A:LEU:HD23	5	0.2
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD11	5	0.2
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD12	5	0.2
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD13	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD21	5	0.2
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD22	5	0.2
(1,1420)	1:131:A:MET:HE3	1:161:A:LEU:HD23	5	0.2
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG2	4	0.2
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG3	4	0.2
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG2	4	0.2
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG3	4	0.2
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG2	4	0.2
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG3	4	0.2
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG2	4	0.2
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG3	4	0.2
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG2	4	0.2
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG3	4	0.2
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG2	4	0.2
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG3	4	0.2
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB2	1	0.2
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB3	1	0.2
(1,1311)	1:101:A:LYS:HD2	1:103:A:SER:H	9	0.2
(1,1311)	1:101:A:LYS:HD3	1:103:A:SER:H	9	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	1	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	1	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	1	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	1	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	1	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	1	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	5	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	5	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	5	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	5	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	5	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	5	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	8	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	8	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	8	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	8	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	8	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	8	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	10	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	10	0.2
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	10	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	10	0.2
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	10	0.2
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	5	0.2
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	5	0.2
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	8	0.2
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	8	0.2
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	5	0.2
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	5	0.2
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	5	0.2
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	5	0.2
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	5	0.2
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	5	0.2
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	7	0.2
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	7	0.2
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	7	0.2
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	7	0.2
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	7	0.2
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	7	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE1	1	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE2	1	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE3	1	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE1	1	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE2	1	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE3	1	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE1	4	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE2	4	0.2
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE3	4	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE1	4	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE2	4	0.2
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE3	4	0.2
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG2	1	0.2
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG3	1	0.2
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB2	9	0.2
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB3	9	0.2
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD2	10	0.2
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD3	10	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD11	6	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD12	6	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD13	6	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD21	6	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD22	6	0.2
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD23	6	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD11	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD12	6	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD13	6	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD21	6	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD22	6	0.2
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD23	6	0.2
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG2	8	0.2
(1,1139)	1:62:A:THR:HG21	1:63:A:GLN:HG3	8	0.2
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG2	8	0.2
(1,1139)	1:62:A:THR:HG22	1:63:A:GLN:HG3	8	0.2
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG2	8	0.2
(1,1139)	1:62:A:THR:HG23	1:63:A:GLN:HG3	8	0.2
(1,1116)	1:54:A:VAL:HG11	1:59:A:PHE:HE1	5	0.2
(1,1116)	1:54:A:VAL:HG11	1:59:A:PHE:HE2	5	0.2
(1,1116)	1:54:A:VAL:HG12	1:59:A:PHE:HE1	5	0.2
(1,1116)	1:54:A:VAL:HG12	1:59:A:PHE:HE2	5	0.2
(1,1116)	1:54:A:VAL:HG13	1:59:A:PHE:HE1	5	0.2
(1,1116)	1:54:A:VAL:HG13	1:59:A:PHE:HE2	5	0.2
(1,1116)	1:54:A:VAL:HG21	1:59:A:PHE:HE1	5	0.2
(1,1116)	1:54:A:VAL:HG21	1:59:A:PHE:HE2	5	0.2
(1,1116)	1:54:A:VAL:HG22	1:59:A:PHE:HE1	5	0.2
(1,1116)	1:54:A:VAL:HG22	1:59:A:PHE:HE2	5	0.2
(1,1116)	1:54:A:VAL:HG23	1:59:A:PHE:HE1	5	0.2
(1,1116)	1:54:A:VAL:HG23	1:59:A:PHE:HE2	5	0.2
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG12	5	0.2
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG13	5	0.2
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG12	5	0.2
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG13	5	0.2
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG12	5	0.2
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG13	5	0.2
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	10	0.2
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	10	0.2
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	10	0.2
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE1	2	0.2
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE2	2	0.2
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE1	10	0.2
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE2	10	0.2
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	10	0.2
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	10	0.2
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	10	0.2
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	10	0.2
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	10	0.2
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	10	0.2
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	10	0.2
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	10	0.2
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	10	0.2
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB1	10	0.2
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB2	10	0.2
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB3	10	0.2
(1,878)	1:92:A:ALA:HA	1:95:A:GLU:HB2	8	0.2
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	1	0.2
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	1	0.2
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	1	0.2
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	1	0.2
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	1	0.2
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	1	0.2
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	8	0.2
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	8	0.2
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	8	0.2
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	8	0.2
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	8	0.2
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	8	0.2
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	4	0.2
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	4	0.2
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	4	0.2
(1,730)	1:90:A:VAL:HG11	1:160:A:LYS:H	4	0.2
(1,730)	1:90:A:VAL:HG12	1:160:A:LYS:H	4	0.2
(1,730)	1:90:A:VAL:HG13	1:160:A:LYS:H	4	0.2
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	4	0.2
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	4	0.2
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	4	0.2
(1,709)	1:98:A:GLU:H	1:99:A:LYS:HD3	10	0.2
(1,640)	1:44:A:LYS:HB2	1:48:A:ASN:H	4	0.2
(1,612)	1:115:A:LEU:H	1:116:A:MET:HB3	1	0.2
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	7	0.2
(1,551)	1:68:A:ILE:HA	1:69:A:SER:H	6	0.2
(1,551)	1:68:A:ILE:HA	1:69:A:SER:H	8	0.2
(1,551)	1:68:A:ILE:HA	1:69:A:SER:H	9	0.2
(1,549)	1:166:A:LYS:HA	1:168:A:GLN:H	1	0.2
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	4	0.2
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	7	0.2
(1,539)	1:151:A:ILE:H	1:152:A:ALA:HA	10	0.2
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	4	0.2
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB1	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB2	7	0.2
(1,295)	1:45:A:ILE:HB	1:82:A:ALA:HB3	7	0.2
(1,189)	1:83:A:ILE:HD11	1:168:A:GLN:HA	2	0.2
(1,189)	1:83:A:ILE:HD12	1:168:A:GLN:HA	2	0.2
(1,189)	1:83:A:ILE:HD13	1:168:A:GLN:HA	2	0.2
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	5	0.2
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	7	0.2
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	7	0.2
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	7	0.2
(1,83)	1:52:A:GLU:H	1:52:A:GLU:HG2	7	0.2
(1,1500)	1:174:A:ASN:HA	1:177:A:GLU:HB2	6	0.19
(1,1500)	1:174:A:ASN:HA	1:177:A:GLU:HB3	6	0.19
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE2	6	0.19
(1,1491)	1:172:A:LEU:HD11	1:173:A:LYS:HE3	6	0.19
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE2	6	0.19
(1,1491)	1:172:A:LEU:HD12	1:173:A:LYS:HE3	6	0.19
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE2	6	0.19
(1,1491)	1:172:A:LEU:HD13	1:173:A:LYS:HE3	6	0.19
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE2	6	0.19
(1,1491)	1:172:A:LEU:HD21	1:173:A:LYS:HE3	6	0.19
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE2	6	0.19
(1,1491)	1:172:A:LEU:HD22	1:173:A:LYS:HE3	6	0.19
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE2	6	0.19
(1,1491)	1:172:A:LEU:HD23	1:173:A:LYS:HE3	6	0.19
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	6	0.19
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	6	0.19
(1,1428)	1:136:A:LYS:HE2	1:137:A:GLU:HA	10	0.19
(1,1428)	1:136:A:LYS:HE3	1:137:A:GLU:HA	10	0.19
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG2	3	0.19
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG3	3	0.19
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG2	3	0.19
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG3	3	0.19
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG2	3	0.19
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG3	3	0.19
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG2	3	0.19
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG3	3	0.19
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG2	3	0.19
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG3	3	0.19
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG2	3	0.19
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG3	3	0.19
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	3	0.19
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	3	0.19
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	3	0.19
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	3	0.19
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	3	0.19
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	3	0.19
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	3	0.19
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	3	0.19
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	3	0.19
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	3	0.19
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	3	0.19
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	4	0.19
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	4	0.19
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	4	0.19
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	4	0.19
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	4	0.19
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	4	0.19
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	4	0.19
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	4	0.19
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	4	0.19
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	4	0.19
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	4	0.19
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	4	0.19
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	9	0.19
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	9	0.19
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	9	0.19
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	9	0.19
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	9	0.19
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	9	0.19
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	3	0.19
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	3	0.19
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE1	7	0.19
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE2	7	0.19
(1,1267)	1:96:A:GLU:HG2	1:112:A:MET:HE3	7	0.19
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE1	7	0.19
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE2	7	0.19
(1,1267)	1:96:A:GLU:HG3	1:112:A:MET:HE3	7	0.19
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB2	8	0.19
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB3	8	0.19
(1,1208)	1:81:A:LYS:H	1:84:A:GLN:HB2	4	0.19
(1,1208)	1:81:A:LYS:H	1:84:A:GLN:HB3	4	0.19
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD11	1	0.19
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD12	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD13	1	0.19
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD21	1	0.19
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD22	1	0.19
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD23	1	0.19
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB2	4	0.19
(1,1161)	1:69:A:SER:HB2	1:70:A:GLU:HB3	4	0.19
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB2	4	0.19
(1,1161)	1:69:A:SER:HB3	1:70:A:GLU:HB3	4	0.19
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG12	4	0.19
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG13	4	0.19
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB1	1	0.19
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB2	1	0.19
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB3	1	0.19
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB1	1	0.19
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB2	1	0.19
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB3	1	0.19
(1,1066)	1:42:A:ILE:HA	1:44:A:LYS:HE2	3	0.19
(1,1066)	1:42:A:ILE:HA	1:44:A:LYS:HE3	3	0.19
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG12	8	0.19
(1,1057)	1:38:A:ILE:HD11	1:42:A:ILE:HG13	8	0.19
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG12	8	0.19
(1,1057)	1:38:A:ILE:HD12	1:42:A:ILE:HG13	8	0.19
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG12	8	0.19
(1,1057)	1:38:A:ILE:HD13	1:42:A:ILE:HG13	8	0.19
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD11	2	0.19
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD12	2	0.19
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD13	2	0.19
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG21	6	0.19
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG22	6	0.19
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG23	6	0.19
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG21	7	0.19
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG22	7	0.19
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG23	7	0.19
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG21	10	0.19
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG22	10	0.19
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG23	10	0.19
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG21	3	0.19
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG22	3	0.19
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG23	3	0.19
(1,878)	1:92:A:ALA:HA	1:95:A:GLU:HB2	2	0.19
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	1	0.19
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	10	0.19
(1,551)	1:68:A:ILE:HA	1:69:A:SER:H	1	0.19
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	6	0.19
(1,461)	1:128:A:ILE:H	1:131:A:MET:H	8	0.19
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	6	0.19
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	6	0.19
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	6	0.19
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	1	0.19
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	1	0.19
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	1	0.19
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE1	1	0.19
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE2	1	0.19
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE3	1	0.19
(1,207)	1:90:A:VAL:HG21	1:154:A:ALA:HA	9	0.19
(1,207)	1:90:A:VAL:HG22	1:154:A:ALA:HA	9	0.19
(1,207)	1:90:A:VAL:HG23	1:154:A:ALA:HA	9	0.19
(1,182)	1:134:A:THR:HB	1:138:A:ALA:HB1	2	0.19
(1,182)	1:134:A:THR:HB	1:138:A:ALA:HB2	2	0.19
(1,182)	1:134:A:THR:HB	1:138:A:ALA:HB3	2	0.19
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	1	0.19
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	1	0.19
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	1	0.19
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	5	0.19
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	5	0.19
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	5	0.19
(1,83)	1:52:A:GLU:H	1:52:A:GLU:HG2	6	0.19
(1,29)	1:102:A:LYS:H	1:102:A:LYS:HG3	2	0.19
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG11	9	0.18
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG12	9	0.18
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG13	9	0.18
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG21	9	0.18
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG22	9	0.18
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG23	9	0.18
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG12	7	0.18
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG13	7	0.18
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG12	9	0.18
(1,1439)	1:145:A:THR:H	1:150:A:ILE:HG13	9	0.18
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG11	3	0.18
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG12	3	0.18
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG13	3	0.18
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG21	3	0.18
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG22	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1408)	1:130:A:LYS:HA	1:164:A:VAL:HG23	3	0.18
(1,1371)	1:123:A:LEU:HD11	1:124:A:GLU:HA	4	0.18
(1,1371)	1:123:A:LEU:HD12	1:124:A:GLU:HA	4	0.18
(1,1371)	1:123:A:LEU:HD13	1:124:A:GLU:HA	4	0.18
(1,1371)	1:123:A:LEU:HD21	1:124:A:GLU:HA	4	0.18
(1,1371)	1:123:A:LEU:HD22	1:124:A:GLU:HA	4	0.18
(1,1371)	1:123:A:LEU:HD23	1:124:A:GLU:HA	4	0.18
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	6	0.18
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	6	0.18
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	6	0.18
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	6	0.18
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	6	0.18
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	6	0.18
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB2	2	0.18
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB3	2	0.18
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB2	5	0.18
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB3	5	0.18
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	6	0.18
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	6	0.18
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG12	10	0.18
(1,1271)	1:97:A:ALA:HB1	1:150:A:ILE:HG13	10	0.18
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG12	10	0.18
(1,1271)	1:97:A:ALA:HB2	1:150:A:ILE:HG13	10	0.18
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG12	10	0.18
(1,1271)	1:97:A:ALA:HB3	1:150:A:ILE:HG13	10	0.18
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG2	2	0.18
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG3	2	0.18
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	1	0.18
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	1	0.18
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	1	0.18
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	1	0.18
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	1	0.18
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	1	0.18
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	3	0.18
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	3	0.18
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	3	0.18
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	3	0.18
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	3	0.18
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	3	0.18
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	3	0.18
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	3	0.18
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	3	0.18
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	3	0.18
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	3	0.18
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	3	0.18
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	3	0.18
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	3	0.18
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	3	0.18
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	3	0.18
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	3	0.18
(1,1152)	1:67:A:LYS:H	1:67:A:LYS:HG2	1	0.18
(1,1152)	1:67:A:LYS:H	1:67:A:LYS:HG3	1	0.18
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG11	8	0.18
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG12	8	0.18
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG13	8	0.18
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG21	8	0.18
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG22	8	0.18
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG23	8	0.18
(1,1091)	1:49:A:ALA:HB1	1:54:A:VAL:HG11	7	0.18
(1,1091)	1:49:A:ALA:HB1	1:54:A:VAL:HG12	7	0.18
(1,1091)	1:49:A:ALA:HB1	1:54:A:VAL:HG13	7	0.18
(1,1091)	1:49:A:ALA:HB1	1:54:A:VAL:HG21	7	0.18
(1,1091)	1:49:A:ALA:HB1	1:54:A:VAL:HG22	7	0.18
(1,1091)	1:49:A:ALA:HB1	1:54:A:VAL:HG23	7	0.18
(1,1091)	1:49:A:ALA:HB2	1:54:A:VAL:HG11	7	0.18
(1,1091)	1:49:A:ALA:HB2	1:54:A:VAL:HG12	7	0.18
(1,1091)	1:49:A:ALA:HB2	1:54:A:VAL:HG13	7	0.18
(1,1091)	1:49:A:ALA:HB2	1:54:A:VAL:HG21	7	0.18
(1,1091)	1:49:A:ALA:HB2	1:54:A:VAL:HG22	7	0.18
(1,1091)	1:49:A:ALA:HB2	1:54:A:VAL:HG23	7	0.18
(1,1091)	1:49:A:ALA:HB3	1:54:A:VAL:HG11	7	0.18
(1,1091)	1:49:A:ALA:HB3	1:54:A:VAL:HG12	7	0.18
(1,1091)	1:49:A:ALA:HB3	1:54:A:VAL:HG13	7	0.18
(1,1091)	1:49:A:ALA:HB3	1:54:A:VAL:HG21	7	0.18
(1,1091)	1:49:A:ALA:HB3	1:54:A:VAL:HG22	7	0.18
(1,1091)	1:49:A:ALA:HB3	1:54:A:VAL:HG23	7	0.18
(1,1042)	1:35:A:ALA:HB1	1:36:A:GLN:HG2	10	0.18
(1,1042)	1:35:A:ALA:HB1	1:36:A:GLN:HG3	10	0.18
(1,1042)	1:35:A:ALA:HB2	1:36:A:GLN:HG2	10	0.18
(1,1042)	1:35:A:ALA:HB2	1:36:A:GLN:HG3	10	0.18
(1,1042)	1:35:A:ALA:HB3	1:36:A:GLN:HG2	10	0.18
(1,1042)	1:35:A:ALA:HB3	1:36:A:GLN:HG3	10	0.18
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	10	0.18
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	10	0.18
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	10	0.18
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	10	0.18
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	10	0.18
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	7	0.18
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	7	0.18
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	7	0.18
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	1	0.18
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	4	0.18
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	4	0.18
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	4	0.18
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	6	0.18
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	6	0.18
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	6	0.18
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG21	3	0.18
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG22	3	0.18
(1,900)	1:58:A:ALA:HB1	1:62:A:THR:HG23	3	0.18
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG21	3	0.18
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG22	3	0.18
(1,900)	1:58:A:ALA:HB2	1:62:A:THR:HG23	3	0.18
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG21	3	0.18
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG22	3	0.18
(1,900)	1:58:A:ALA:HB3	1:62:A:THR:HG23	3	0.18
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	3	0.18
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	3	0.18
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	3	0.18
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	3	0.18
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	3	0.18
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	3	0.18
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	3	0.18
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	3	0.18
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	3	0.18
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD1	2	0.18
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD2	2	0.18
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD1	2	0.18
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD2	2	0.18
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD1	2	0.18
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD2	2	0.18
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD1	3	0.18
(1,833)	1:49:A:ALA:HB1	1:74:A:PHE:HD2	3	0.18
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD1	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:49:A:ALA:HB2	1:74:A:PHE:HD2	3	0.18
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD1	3	0.18
(1,833)	1:49:A:ALA:HB3	1:74:A:PHE:HD2	3	0.18
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	10	0.18
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	10	0.18
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	10	0.18
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	1	0.18
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	1	0.18
(1,684)	1:179:A:ALA:HB1	1:180:A:LYS:H	7	0.18
(1,684)	1:179:A:ALA:HB2	1:180:A:LYS:H	7	0.18
(1,684)	1:179:A:ALA:HB3	1:180:A:LYS:H	7	0.18
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	2	0.18
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	2	0.18
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	7	0.18
(1,579)	1:132:A:THR:HB	1:133:A:GLY:H	6	0.18
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	3	0.18
(1,552)	1:29:A:ILE:H	1:30:A:ARG:HA	1	0.18
(1,551)	1:68:A:ILE:HA	1:69:A:SER:H	4	0.18
(1,533)	1:49:A:ALA:H	1:50:A:LYS:HA	6	0.18
(1,455)	1:59:A:PHE:H	1:61:A:ASN:H	10	0.18
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG21	6	0.18
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG22	6	0.18
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG23	6	0.18
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD11	4	0.18
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD12	4	0.18
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD13	4	0.18
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG21	2	0.18
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG22	2	0.18
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG23	2	0.18
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG21	2	0.18
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG22	2	0.18
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG23	2	0.18
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG21	2	0.18
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG22	2	0.18
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG23	2	0.18
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG21	8	0.18
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG22	8	0.18
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG23	8	0.18
(1,288)	1:115:A:LEU:HB3	1:119:A:VAL:HB	1	0.18
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG21	3	0.18
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG22	3	0.18
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG23	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:113:A:TYR:HD1	1:116:A:MET:HE1	2	0.18
(1,139)	1:113:A:TYR:HD1	1:116:A:MET:HE2	2	0.18
(1,139)	1:113:A:TYR:HD1	1:116:A:MET:HE3	2	0.18
(1,139)	1:113:A:TYR:HD2	1:116:A:MET:HE1	2	0.18
(1,139)	1:113:A:TYR:HD2	1:116:A:MET:HE2	2	0.18
(1,139)	1:113:A:TYR:HD2	1:116:A:MET:HE3	2	0.18
(1,134)	1:140:A:GLN:H	1:140:A:GLN:HG2	1	0.18
(1,83)	1:52:A:GLU:H	1:52:A:GLU:HG2	8	0.18
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD11	5	0.18
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD12	5	0.18
(1,47)	1:144:A:ALA:H	1:150:A:ILE:HD13	5	0.18
(1,1495)	1:173:A:LYS:HA	1:173:A:LYS:HE2	6	0.17
(1,1495)	1:173:A:LYS:HA	1:173:A:LYS:HE3	6	0.17
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG12	7	0.17
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG13	7	0.17
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG12	10	0.17
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG13	10	0.17
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB2	5	0.17
(1,1436)	1:142:A:THR:HG21	1:143:A:PRO:HB3	5	0.17
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB2	5	0.17
(1,1436)	1:142:A:THR:HG22	1:143:A:PRO:HB3	5	0.17
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB2	5	0.17
(1,1436)	1:142:A:THR:HG23	1:143:A:PRO:HB3	5	0.17
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE1	8	0.17
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE2	8	0.17
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE3	8	0.17
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE1	8	0.17
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE2	8	0.17
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE3	8	0.17
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD11	7	0.17
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD12	7	0.17
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD13	7	0.17
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD11	7	0.17
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD12	7	0.17
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD13	7	0.17
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	1	0.17
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	1	0.17
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	1	0.17
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	1	0.17
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	1	0.17
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	1	0.17
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	1	0.17
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	1	0.17
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	1	0.17
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	1	0.17
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	1	0.17
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	2	0.17
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	2	0.17
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	2	0.17
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	2	0.17
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	2	0.17
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	2	0.17
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	2	0.17
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	2	0.17
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	2	0.17
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	2	0.17
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	2	0.17
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	2	0.17
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB2	9	0.17
(1,1372)	1:123:A:LEU:HD11	1:124:A:GLU:HB3	9	0.17
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB2	9	0.17
(1,1372)	1:123:A:LEU:HD12	1:124:A:GLU:HB3	9	0.17
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB2	9	0.17
(1,1372)	1:123:A:LEU:HD13	1:124:A:GLU:HB3	9	0.17
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB2	9	0.17
(1,1372)	1:123:A:LEU:HD21	1:124:A:GLU:HB3	9	0.17
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB2	9	0.17
(1,1372)	1:123:A:LEU:HD22	1:124:A:GLU:HB3	9	0.17
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB2	9	0.17
(1,1372)	1:123:A:LEU:HD23	1:124:A:GLU:HB3	9	0.17
(1,1371)	1:123:A:LEU:HD11	1:124:A:GLU:HA	3	0.17
(1,1371)	1:123:A:LEU:HD12	1:124:A:GLU:HA	3	0.17
(1,1371)	1:123:A:LEU:HD13	1:124:A:GLU:HA	3	0.17
(1,1371)	1:123:A:LEU:HD21	1:124:A:GLU:HA	3	0.17
(1,1371)	1:123:A:LEU:HD22	1:124:A:GLU:HA	3	0.17
(1,1371)	1:123:A:LEU:HD23	1:124:A:GLU:HA	3	0.17
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	8	0.17
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	8	0.17
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	8	0.17
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	8	0.17
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	8	0.17
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	8	0.17
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB3	2	0.17
(1,1320)	1:105:A:SER:H	1:105:A:SER:HB2	7	0.17
(1,1320)	1:105:A:SER:H	1:105:A:SER:HB3	7	0.17
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD2	9	0.17
(1,1273)	1:98:A:GLU:H	1:99:A:LYS:HD3	9	0.17
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG2	10	0.17
(1,1263)	1:96:A:GLU:HA	1:99:A:LYS:HG3	10	0.17
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB1	8	0.17
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB2	8	0.17
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB3	8	0.17
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB1	8	0.17
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB2	8	0.17
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB3	8	0.17
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB1	3	0.17
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB2	3	0.17
(1,1236)	1:88:A:ARG:HB2	1:92:A:ALA:HB3	3	0.17
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB1	3	0.17
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB2	3	0.17
(1,1236)	1:88:A:ARG:HB3	1:92:A:ALA:HB3	3	0.17
(1,1222)	1:85:A:VAL:HG11	1:126:A:ILE:HG21	6	0.17
(1,1222)	1:85:A:VAL:HG11	1:126:A:ILE:HG22	6	0.17
(1,1222)	1:85:A:VAL:HG11	1:126:A:ILE:HG23	6	0.17
(1,1222)	1:85:A:VAL:HG12	1:126:A:ILE:HG21	6	0.17
(1,1222)	1:85:A:VAL:HG12	1:126:A:ILE:HG22	6	0.17
(1,1222)	1:85:A:VAL:HG12	1:126:A:ILE:HG23	6	0.17
(1,1222)	1:85:A:VAL:HG13	1:126:A:ILE:HG21	6	0.17
(1,1222)	1:85:A:VAL:HG13	1:126:A:ILE:HG22	6	0.17
(1,1222)	1:85:A:VAL:HG13	1:126:A:ILE:HG23	6	0.17
(1,1222)	1:85:A:VAL:HG21	1:126:A:ILE:HG21	6	0.17
(1,1222)	1:85:A:VAL:HG21	1:126:A:ILE:HG22	6	0.17
(1,1222)	1:85:A:VAL:HG21	1:126:A:ILE:HG23	6	0.17
(1,1222)	1:85:A:VAL:HG22	1:126:A:ILE:HG21	6	0.17
(1,1222)	1:85:A:VAL:HG22	1:126:A:ILE:HG22	6	0.17
(1,1222)	1:85:A:VAL:HG22	1:126:A:ILE:HG23	6	0.17
(1,1222)	1:85:A:VAL:HG23	1:126:A:ILE:HG21	6	0.17
(1,1222)	1:85:A:VAL:HG23	1:126:A:ILE:HG22	6	0.17
(1,1222)	1:85:A:VAL:HG23	1:126:A:ILE:HG23	6	0.17
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD2	8	0.17
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD3	8	0.17
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD11	3	0.17
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD12	3	0.17
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD21	3	0.17
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD22	3	0.17
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD23	3	0.17
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG12	5	0.17
(1,1136)	1:59:A:PHE:HB3	1:75:A:ILE:HG13	5	0.17
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG2	3	0.17
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG3	3	0.17
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG2	7	0.17
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG3	7	0.17
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	7	0.17
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	7	0.17
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	7	0.17
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	7	0.17
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	7	0.17
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	7	0.17
(1,1023)	1:27:A:THR:H	1:28:A:LYS:HG2	1	0.17
(1,1023)	1:27:A:THR:H	1:28:A:LYS:HG3	1	0.17
(1,983)	1:35:A:ALA:HA	1:38:A:ILE:HB	1	0.17
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD1	5	0.17
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD2	5	0.17
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD11	10	0.17
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD12	10	0.17
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD13	10	0.17
(1,941)	1:131:A:MET:HE1	1:162:A:ASN:H	7	0.17
(1,941)	1:131:A:MET:HE2	1:162:A:ASN:H	7	0.17
(1,941)	1:131:A:MET:HE3	1:162:A:ASN:H	7	0.17
(1,878)	1:92:A:ALA:HA	1:95:A:GLU:HB2	5	0.17
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD11	6	0.17
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD12	6	0.17
(1,808)	1:149:A:GLY:H	1:150:A:ILE:HD13	6	0.17
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD21	3	0.17
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD22	3	0.17
(1,769)	1:171:A:ALA:H	1:172:A:LEU:HD23	3	0.17
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	2	0.17
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	2	0.17
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	8	0.17
(1,598)	1:61:A:ASN:HB2	1:63:A:GLN:H	1	0.17
(1,579)	1:132:A:THR:HB	1:133:A:GLY:H	5	0.17
(1,579)	1:132:A:THR:HB	1:133:A:GLY:H	10	0.17
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG21	8	0.17
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG22	8	0.17
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG23	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:29:A:ILE:HB	1:30:A:ARG:HA	8	0.17
(1,168)	1:151:A:ILE:HB	1:152:A:ALA:HA	6	0.17
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	3	0.17
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	3	0.17
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	3	0.17
(1,93)	1:91:A:LYS:HG2	1:93:A:ILE:H	5	0.17
(1,93)	1:91:A:LYS:HG3	1:93:A:ILE:H	5	0.17
(1,83)	1:52:A:GLU:H	1:52:A:GLU:HG2	2	0.17
(1,83)	1:52:A:GLU:H	1:52:A:GLU:HG2	5	0.17
(1,1515)	1:177:A:GLU:HG2	1:179:A:ALA:H	7	0.16
(1,1515)	1:177:A:GLU:HG3	1:179:A:ALA:H	7	0.16
(1,1498)	1:173:A:LYS:HG2	1:174:A:ASN:H	4	0.16
(1,1498)	1:173:A:LYS:HG3	1:174:A:ASN:H	4	0.16
(1,1482)	1:170:A:ASP:HA	1:173:A:LYS:HG2	7	0.16
(1,1482)	1:170:A:ASP:HA	1:173:A:LYS:HG3	7	0.16
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	5	0.16
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	5	0.16
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD11	5	0.16
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD12	5	0.16
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD13	5	0.16
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD11	5	0.16
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD12	5	0.16
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD13	5	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	1	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	1	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	1	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	1	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	1	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	1	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	2	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	2	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	2	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	2	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	2	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	2	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	7	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	7	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	7	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	7	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	7	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	7	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	9	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	9	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	9	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	9	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	9	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE1	10	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE2	10	0.16
(1,1350)	1:116:A:MET:HB2	1:116:A:MET:HE3	10	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE1	10	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE2	10	0.16
(1,1350)	1:116:A:MET:HB3	1:116:A:MET:HE3	10	0.16
(1,1347)	1:115:A:LEU:HD11	1:119:A:VAL:HB	4	0.16
(1,1347)	1:115:A:LEU:HD12	1:119:A:VAL:HB	4	0.16
(1,1347)	1:115:A:LEU:HD13	1:119:A:VAL:HB	4	0.16
(1,1347)	1:115:A:LEU:HD21	1:119:A:VAL:HB	4	0.16
(1,1347)	1:115:A:LEU:HD22	1:119:A:VAL:HB	4	0.16
(1,1347)	1:115:A:LEU:HD23	1:119:A:VAL:HB	4	0.16
(1,1326)	1:109:A:PHE:HB2	1:112:A:MET:HE1	2	0.16
(1,1326)	1:109:A:PHE:HB2	1:112:A:MET:HE2	2	0.16
(1,1326)	1:109:A:PHE:HB2	1:112:A:MET:HE3	2	0.16
(1,1326)	1:109:A:PHE:HB3	1:112:A:MET:HE1	2	0.16
(1,1326)	1:109:A:PHE:HB3	1:112:A:MET:HE2	2	0.16
(1,1326)	1:109:A:PHE:HB3	1:112:A:MET:HE3	2	0.16
(1,1321)	1:105:A:SER:HB2	1:106:A:SER:H	2	0.16
(1,1321)	1:105:A:SER:HB3	1:106:A:SER:H	2	0.16
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG21	8	0.16
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG22	8	0.16
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG23	8	0.16
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG21	8	0.16
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG22	8	0.16
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG23	8	0.16
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG21	8	0.16
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG22	8	0.16
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG23	8	0.16
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG21	8	0.16
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG22	8	0.16
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG23	8	0.16
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG21	8	0.16
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG22	8	0.16
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG23	8	0.16
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG21	8	0.16
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG22	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG23	8	0.16
(1,1291)	1:100:A:LEU:HB2	1:146:A:THR:HG21	5	0.16
(1,1291)	1:100:A:LEU:HB2	1:146:A:THR:HG22	5	0.16
(1,1291)	1:100:A:LEU:HB2	1:146:A:THR:HG23	5	0.16
(1,1291)	1:100:A:LEU:HB3	1:146:A:THR:HG21	5	0.16
(1,1291)	1:100:A:LEU:HB3	1:146:A:THR:HG22	5	0.16
(1,1291)	1:100:A:LEU:HB3	1:146:A:THR:HG23	5	0.16
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB1	6	0.16
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB2	6	0.16
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB3	6	0.16
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB1	6	0.16
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB2	6	0.16
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB3	6	0.16
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD11	6	0.16
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD12	6	0.16
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD13	6	0.16
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD11	6	0.16
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD12	6	0.16
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD13	6	0.16
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD11	6	0.16
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD12	6	0.16
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD13	6	0.16
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD11	6	0.16
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD12	6	0.16
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD13	6	0.16
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD11	6	0.16
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD12	6	0.16
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD13	6	0.16
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD11	6	0.16
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD12	6	0.16
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD13	6	0.16
(1,1184)	1:74:A:PHE:H	1:75:A:ILE:HG12	10	0.16
(1,1184)	1:74:A:PHE:H	1:75:A:ILE:HG13	10	0.16
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG2	2	0.16
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG3	2	0.16
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG2	6	0.16
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG3	6	0.16
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG2	8	0.16
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG3	8	0.16
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD11	9	0.16
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD12	9	0.16
(1,1055)	1:38:A:ILE:HG12	1:42:A:ILE:HD13	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD11	9	0.16
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD12	9	0.16
(1,1055)	1:38:A:ILE:HG13	1:42:A:ILE:HD13	9	0.16
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	3	0.16
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	3	0.16
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	3	0.16
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	3	0.16
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	3	0.16
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	3	0.16
(1,1030)	1:28:A:LYS:HA	1:28:A:LYS:HD2	7	0.16
(1,1030)	1:28:A:LYS:HA	1:28:A:LYS:HD3	7	0.16
(1,1004)	1:45:A:ILE:HD11	1:74:A:PHE:HD1	2	0.16
(1,1004)	1:45:A:ILE:HD11	1:74:A:PHE:HD2	2	0.16
(1,1004)	1:45:A:ILE:HD12	1:74:A:PHE:HD1	2	0.16
(1,1004)	1:45:A:ILE:HD12	1:74:A:PHE:HD2	2	0.16
(1,1004)	1:45:A:ILE:HD13	1:74:A:PHE:HD1	2	0.16
(1,1004)	1:45:A:ILE:HD13	1:74:A:PHE:HD2	2	0.16
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE1	10	0.16
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE2	10	0.16
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	2	0.16
(1,943)	1:136:A:LYS:H	1:137:A:GLU:HA	9	0.16
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG21	2	0.16
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG22	2	0.16
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG23	2	0.16
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	7	0.16
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	7	0.16
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	7	0.16
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	7	0.16
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	7	0.16
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	7	0.16
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	7	0.16
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	7	0.16
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	7	0.16
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB1	6	0.16
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB2	6	0.16
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB3	6	0.16
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	4	0.16
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	4	0.16
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	4	0.16
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	4	0.16
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	4	0.16
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	6	0.16
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	6	0.16
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	6	0.16
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	1	0.16
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	1	0.16
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	1	0.16
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	1	0.16
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	1	0.16
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	1	0.16
(1,640)	1:44:A:LYS:HB2	1:48:A:ASN:H	5	0.16
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	3	0.16
(1,571)	1:158:A:GLU:HA	1:162:A:ASN:H	2	0.16
(1,564)	1:163:A:ASN:H	1:164:A:VAL:HA	8	0.16
(1,556)	1:24:A:THR:HB	1:25:A:GLY:H	2	0.16
(1,537)	1:68:A:ILE:HA	1:70:A:GLU:H	8	0.16
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	2	0.16
(1,533)	1:49:A:ALA:H	1:50:A:LYS:HA	10	0.16
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE1	1	0.16
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE2	1	0.16
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE3	1	0.16
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE1	1	0.16
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE2	1	0.16
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE3	1	0.16
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE1	1	0.16
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE2	1	0.16
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE3	1	0.16
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE1	2	0.16
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE2	2	0.16
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE3	2	0.16
(1,257)	1:59:A:PHE:HB2	1:60:A:THR:HA	9	0.16
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG21	9	0.16
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG22	9	0.16
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG23	9	0.16
(1,238)	1:56:A:PHE:HA	1:59:A:PHE:HB3	9	0.16
(1,204)	1:97:A:ALA:HA	1:100:A:LEU:HG	2	0.16
(1,180)	1:58:A:ALA:HB1	1:62:A:THR:HB	10	0.16
(1,180)	1:58:A:ALA:HB2	1:62:A:THR:HB	10	0.16
(1,180)	1:58:A:ALA:HB3	1:62:A:THR:HB	10	0.16
(1,171)	1:115:A:LEU:HA	1:117:A:ILE:HB	1	0.16
(1,1513)	1:177:A:GLU:HG2	1:178:A:LYS:H	4	0.15
(1,1513)	1:177:A:GLU:HG3	1:178:A:LYS:H	4	0.15
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE1	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE2	10	0.15
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE3	10	0.15
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE1	10	0.15
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE2	10	0.15
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE3	10	0.15
(1,1446)	1:150:A:ILE:HG12	1:151:A:ILE:H	2	0.15
(1,1446)	1:150:A:ILE:HG13	1:151:A:ILE:H	2	0.15
(1,1400)	1:128:A:ILE:HG12	1:129:A:GLN:H	7	0.15
(1,1400)	1:128:A:ILE:HG13	1:129:A:GLN:H	7	0.15
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG2	2	0.15
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG3	2	0.15
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG2	2	0.15
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG3	2	0.15
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG2	2	0.15
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG3	2	0.15
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG2	2	0.15
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG3	2	0.15
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG2	2	0.15
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG3	2	0.15
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG2	2	0.15
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG3	2	0.15
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD2	9	0.15
(1,1299)	1:101:A:LYS:H	1:101:A:LYS:HD3	9	0.15
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG21	2	0.15
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG22	2	0.15
(1,1297)	1:100:A:LEU:HD11	1:146:A:THR:HG23	2	0.15
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG21	2	0.15
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG22	2	0.15
(1,1297)	1:100:A:LEU:HD12	1:146:A:THR:HG23	2	0.15
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG21	2	0.15
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG22	2	0.15
(1,1297)	1:100:A:LEU:HD13	1:146:A:THR:HG23	2	0.15
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG21	2	0.15
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG22	2	0.15
(1,1297)	1:100:A:LEU:HD21	1:146:A:THR:HG23	2	0.15
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG21	2	0.15
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG22	2	0.15
(1,1297)	1:100:A:LEU:HD22	1:146:A:THR:HG23	2	0.15
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG21	2	0.15
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG22	2	0.15
(1,1297)	1:100:A:LEU:HD23	1:146:A:THR:HG23	2	0.15
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB1	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB2	4	0.15
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB3	4	0.15
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB1	4	0.15
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB2	4	0.15
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB3	4	0.15
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD11	5	0.15
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD12	5	0.15
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD13	5	0.15
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD21	5	0.15
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD22	5	0.15
(1,1282)	1:99:A:LYS:H	1:100:A:LEU:HD23	5	0.15
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG21	2	0.15
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG22	2	0.15
(1,1277)	1:98:A:GLU:HG2	1:151:A:ILE:HG23	2	0.15
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG21	2	0.15
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG22	2	0.15
(1,1277)	1:98:A:GLU:HG3	1:151:A:ILE:HG23	2	0.15
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD11	2	0.15
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD12	2	0.15
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD13	2	0.15
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD21	2	0.15
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD22	2	0.15
(1,1182)	1:73:A:GLU:HG2	1:172:A:LEU:HD23	2	0.15
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD11	2	0.15
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD12	2	0.15
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD13	2	0.15
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD21	2	0.15
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD22	2	0.15
(1,1182)	1:73:A:GLU:HG3	1:172:A:LEU:HD23	2	0.15
(1,1143)	1:63:A:GLN:H	1:63:A:GLN:HG2	2	0.15
(1,1143)	1:63:A:GLN:H	1:63:A:GLN:HG3	2	0.15
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG11	6	0.15
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG12	6	0.15
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG13	6	0.15
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG21	6	0.15
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG22	6	0.15
(1,1110)	1:53:A:GLY:HA2	1:54:A:VAL:HG23	6	0.15
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG2	5	0.15
(1,1105)	1:52:A:GLU:H	1:52:A:GLU:HG3	5	0.15
(1,1031)	1:28:A:LYS:HB2	1:29:A:ILE:HG12	5	0.15
(1,1031)	1:28:A:LYS:HB2	1:29:A:ILE:HG13	5	0.15
(1,1031)	1:28:A:LYS:HB3	1:29:A:ILE:HG12	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	1:28:A:LYS:HB3	1:29:A:ILE:HG13	5	0.15
(1,1022)	1:27:A:THR:H	1:28:A:LYS:HB2	1	0.15
(1,1022)	1:27:A:THR:H	1:28:A:LYS:HB3	1	0.15
(1,1022)	1:27:A:THR:H	1:28:A:LYS:HB2	7	0.15
(1,1022)	1:27:A:THR:H	1:28:A:LYS:HB3	7	0.15
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE1	8	0.15
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE2	8	0.15
(1,950)	1:116:A:MET:HE1	1:117:A:ILE:H	6	0.15
(1,950)	1:116:A:MET:HE2	1:117:A:ILE:H	6	0.15
(1,950)	1:116:A:MET:HE3	1:117:A:ILE:H	6	0.15
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG21	1	0.15
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG22	1	0.15
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG23	1	0.15
(1,886)	1:64:A:THR:HG21	1:67:A:LYS:HB3	7	0.15
(1,886)	1:64:A:THR:HG22	1:67:A:LYS:HB3	7	0.15
(1,886)	1:64:A:THR:HG23	1:67:A:LYS:HB3	7	0.15
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB1	5	0.15
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB2	5	0.15
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB3	5	0.15
(1,837)	1:113:A:TYR:HE1	1:139:A:ALA:HB1	3	0.15
(1,837)	1:113:A:TYR:HE1	1:139:A:ALA:HB2	3	0.15
(1,837)	1:113:A:TYR:HE1	1:139:A:ALA:HB3	3	0.15
(1,837)	1:113:A:TYR:HE2	1:139:A:ALA:HB1	3	0.15
(1,837)	1:113:A:TYR:HE2	1:139:A:ALA:HB2	3	0.15
(1,837)	1:113:A:TYR:HE2	1:139:A:ALA:HB3	3	0.15
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	5	0.15
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	5	0.15
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	5	0.15
(1,799)	1:45:A:ILE:HD11	1:79:A:LYS:H	6	0.15
(1,799)	1:45:A:ILE:HD12	1:79:A:LYS:H	6	0.15
(1,799)	1:45:A:ILE:HD13	1:79:A:LYS:H	6	0.15
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	2	0.15
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	2	0.15
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	2	0.15
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB1	9	0.15
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB2	9	0.15
(1,741)	1:79:A:LYS:H	1:82:A:ALA:HB3	9	0.15
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	9	0.15
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	9	0.15
(1,591)	1:55:A:LYS:HE3	1:58:A:ALA:H	4	0.15
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG21	8	0.15
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG22	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG23	8	0.15
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG21	10	0.15
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG22	10	0.15
(1,340)	1:124:A:GLU:HA	1:126:A:ILE:HG23	10	0.15
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG21	10	0.15
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG22	10	0.15
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG23	10	0.15
(1,288)	1:115:A:LEU:HB3	1:119:A:VAL:HB	6	0.15
(1,253)	1:101:A:LYS:HE3	1:151:A:ILE:HD11	6	0.15
(1,253)	1:101:A:LYS:HE3	1:151:A:ILE:HD12	6	0.15
(1,253)	1:101:A:LYS:HE3	1:151:A:ILE:HD13	6	0.15
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG21	3	0.15
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG22	3	0.15
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG23	3	0.15
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG21	9	0.15
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG22	9	0.15
(1,244)	1:61:A:ASN:HB2	1:62:A:THR:HG23	9	0.15
(1,204)	1:97:A:ALA:HA	1:100:A:LEU:HG	7	0.15
(1,69)	1:88:A:ARG:HD3	1:92:A:ALA:H	4	0.15
(1,31)	1:131:A:MET:HE1	1:161:A:LEU:H	4	0.15
(1,31)	1:131:A:MET:HE2	1:161:A:LEU:H	4	0.15
(1,31)	1:131:A:MET:HE3	1:161:A:LEU:H	4	0.15
(1,1495)	1:173:A:LYS:HA	1:173:A:LYS:HE2	5	0.14
(1,1495)	1:173:A:LYS:HA	1:173:A:LYS:HE3	5	0.14
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE1	1	0.14
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE2	1	0.14
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE3	1	0.14
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE1	1	0.14
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE2	1	0.14
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE3	1	0.14
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE1	3	0.14
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE2	3	0.14
(1,1450)	1:155:A:GLN:HG2	1:157:A:MET:HE3	3	0.14
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE1	3	0.14
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE2	3	0.14
(1,1450)	1:155:A:GLN:HG3	1:157:A:MET:HE3	3	0.14
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG12	4	0.14
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG13	4	0.14
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE1	3	0.14
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE2	3	0.14
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE3	3	0.14
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE1	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE2	3	0.14
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE3	3	0.14
(1,1400)	1:128:A:ILE:HG12	1:129:A:GLN:H	5	0.14
(1,1400)	1:128:A:ILE:HG13	1:129:A:GLN:H	5	0.14
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE1	8	0.14
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE2	8	0.14
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE3	8	0.14
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE1	8	0.14
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE2	8	0.14
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE3	8	0.14
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB2	2	0.14
(1,1247)	1:92:A:ALA:HA	1:95:A:GLU:HB3	2	0.14
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD2	5	0.14
(1,1215)	1:85:A:VAL:HA	1:88:A:ARG:HD3	5	0.14
(1,1200)	1:76:A:LEU:HD11	1:77:A:LYS:H	1	0.14
(1,1200)	1:76:A:LEU:HD12	1:77:A:LYS:H	1	0.14
(1,1200)	1:76:A:LEU:HD13	1:77:A:LYS:H	1	0.14
(1,1200)	1:76:A:LEU:HD21	1:77:A:LYS:H	1	0.14
(1,1200)	1:76:A:LEU:HD22	1:77:A:LYS:H	1	0.14
(1,1200)	1:76:A:LEU:HD23	1:77:A:LYS:H	1	0.14
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	8	0.14
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	8	0.14
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	8	0.14
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	8	0.14
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	8	0.14
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	8	0.14
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG12	3	0.14
(1,1155)	1:67:A:LYS:HB2	1:68:A:ILE:HG13	3	0.14
(1,1041)	1:35:A:ALA:HB1	1:36:A:GLN:HB2	1	0.14
(1,1041)	1:35:A:ALA:HB1	1:36:A:GLN:HB3	1	0.14
(1,1041)	1:35:A:ALA:HB2	1:36:A:GLN:HB2	1	0.14
(1,1041)	1:35:A:ALA:HB2	1:36:A:GLN:HB3	1	0.14
(1,1041)	1:35:A:ALA:HB3	1:36:A:GLN:HB2	1	0.14
(1,1041)	1:35:A:ALA:HB3	1:36:A:GLN:HB3	1	0.14
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD11	8	0.14
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD12	8	0.14
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD13	8	0.14
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD21	8	0.14
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD22	8	0.14
(1,1040)	1:35:A:ALA:HA	1:115:A:LEU:HD23	8	0.14
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	3	0.14
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	3	0.14
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	3	0.14
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	5	0.14
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	5	0.14
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	5	0.14
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	5	0.14
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB2	8	0.14
(1,1012)	1:22:A:GLY:HA2	1:23:A:LEU:HB3	8	0.14
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB2	8	0.14
(1,1012)	1:22:A:GLY:HA3	1:23:A:LEU:HB3	8	0.14
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE1	4	0.14
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE2	4	0.14
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG21	10	0.14
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG22	10	0.14
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG23	10	0.14
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	8	0.14
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	8	0.14
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	8	0.14
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	8	0.14
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	8	0.14
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	8	0.14
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	8	0.14
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	8	0.14
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	8	0.14
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	9	0.14
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	9	0.14
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	9	0.14
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	9	0.14
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	9	0.14
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	9	0.14
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	9	0.14
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	9	0.14
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	9	0.14
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG21	8	0.14
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG22	8	0.14
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG23	8	0.14
(1,886)	1:64:A:THR:HG21	1:67:A:LYS:HB3	8	0.14
(1,886)	1:64:A:THR:HG22	1:67:A:LYS:HB3	8	0.14
(1,886)	1:64:A:THR:HG23	1:67:A:LYS:HB3	8	0.14
(1,886)	1:64:A:THR:HG21	1:67:A:LYS:HB3	10	0.14
(1,886)	1:64:A:THR:HG22	1:67:A:LYS:HB3	10	0.14
(1,886)	1:64:A:THR:HG23	1:67:A:LYS:HB3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB1	7	0.14
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB2	7	0.14
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB3	7	0.14
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG21	5	0.14
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG22	5	0.14
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG23	5	0.14
(1,840)	1:113:A:TYR:HE1	1:135:A:VAL:HA	5	0.14
(1,840)	1:113:A:TYR:HE2	1:135:A:VAL:HA	5	0.14
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD11	9	0.14
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD12	9	0.14
(1,781)	1:82:A:ALA:H	1:83:A:ILE:HD13	9	0.14
(1,765)	1:150:A:ILE:HG21	1:153:A:ILE:H	4	0.14
(1,765)	1:150:A:ILE:HG22	1:153:A:ILE:H	4	0.14
(1,765)	1:150:A:ILE:HG23	1:153:A:ILE:H	4	0.14
(1,715)	1:53:A:GLY:H	1:54:A:VAL:HB	4	0.14
(1,709)	1:98:A:GLU:H	1:99:A:LYS:HD3	7	0.14
(1,639)	1:160:A:LYS:H	1:161:A:LEU:HG	5	0.14
(1,625)	1:140:A:GLN:HB3	1:142:A:THR:H	8	0.14
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	1	0.14
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	5	0.14
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	8	0.14
(1,551)	1:68:A:ILE:HA	1:69:A:SER:H	3	0.14
(1,533)	1:49:A:ALA:H	1:50:A:LYS:HA	1	0.14
(1,530)	1:61:A:ASN:HA	1:62:A:THR:H	2	0.14
(1,488)	1:105:A:SER:H	1:106:A:SER:H	10	0.14
(1,408)	1:25:A:GLY:H	1:26:A:GLU:H	4	0.14
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD11	1	0.14
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD12	1	0.14
(1,369)	1:76:A:LEU:HG	1:80:A:ILE:HD13	1	0.14
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	10	0.14
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	10	0.14
(1,358)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	10	0.14
(1,257)	1:59:A:PHE:HB2	1:60:A:THR:HA	1	0.14
(1,257)	1:59:A:PHE:HB2	1:60:A:THR:HA	4	0.14
(1,257)	1:59:A:PHE:HB2	1:60:A:THR:HA	6	0.14
(1,207)	1:90:A:VAL:HG21	1:154:A:ALA:HA	4	0.14
(1,207)	1:90:A:VAL:HG22	1:154:A:ALA:HA	4	0.14
(1,207)	1:90:A:VAL:HG23	1:154:A:ALA:HA	4	0.14
(1,189)	1:83:A:ILE:HD11	1:168:A:GLN:HA	9	0.14
(1,189)	1:83:A:ILE:HD12	1:168:A:GLN:HA	9	0.14
(1,189)	1:83:A:ILE:HD13	1:168:A:GLN:HA	9	0.14
(1,168)	1:151:A:ILE:HB	1:152:A:ALA:HA	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG21	7	0.14
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG22	7	0.14
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG23	7	0.14
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	8	0.14
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	10	0.14
(1,1493)	1:173:A:LYS:HA	1:173:A:LYS:HG2	6	0.13
(1,1493)	1:173:A:LYS:HA	1:173:A:LYS:HG3	6	0.13
(1,1462)	1:161:A:LEU:HD11	1:165:A:ASN:H	7	0.13
(1,1462)	1:161:A:LEU:HD12	1:165:A:ASN:H	7	0.13
(1,1462)	1:161:A:LEU:HD13	1:165:A:ASN:H	7	0.13
(1,1462)	1:161:A:LEU:HD21	1:165:A:ASN:H	7	0.13
(1,1462)	1:161:A:LEU:HD22	1:165:A:ASN:H	7	0.13
(1,1462)	1:161:A:LEU:HD23	1:165:A:ASN:H	7	0.13
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD2	9	0.13
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD3	9	0.13
(1,1428)	1:136:A:LYS:HE2	1:137:A:GLU:HA	5	0.13
(1,1428)	1:136:A:LYS:HE3	1:137:A:GLU:HA	5	0.13
(1,1400)	1:128:A:ILE:HG12	1:129:A:GLN:H	10	0.13
(1,1400)	1:128:A:ILE:HG13	1:129:A:GLN:H	10	0.13
(1,1347)	1:115:A:LEU:HD11	1:119:A:VAL:HB	2	0.13
(1,1347)	1:115:A:LEU:HD12	1:119:A:VAL:HB	2	0.13
(1,1347)	1:115:A:LEU:HD13	1:119:A:VAL:HB	2	0.13
(1,1347)	1:115:A:LEU:HD21	1:119:A:VAL:HB	2	0.13
(1,1347)	1:115:A:LEU:HD22	1:119:A:VAL:HB	2	0.13
(1,1347)	1:115:A:LEU:HD23	1:119:A:VAL:HB	2	0.13
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB2	9	0.13
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB3	9	0.13
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB2	3	0.13
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB3	3	0.13
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE1	2	0.13
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE2	2	0.13
(1,1253)	1:94:A:LYS:HG2	1:157:A:MET:HE3	2	0.13
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE1	2	0.13
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE2	2	0.13
(1,1253)	1:94:A:LYS:HG3	1:157:A:MET:HE3	2	0.13
(1,1239)	1:88:A:ARG:HD2	1:89:A:PHE:H	10	0.13
(1,1239)	1:88:A:ARG:HD3	1:89:A:PHE:H	10	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	4	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	4	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	4	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	4	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	4	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	4	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	4	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	4	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	4	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	4	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	4	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	4	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	4	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	4	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	4	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	4	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	4	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	6	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	6	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	6	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	6	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	6	0.13
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	6	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	6	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	6	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	6	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	6	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	6	0.13
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	6	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	6	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	6	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	6	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	6	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	6	0.13
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	6	0.13
(1,1031)	1:28:A:LYS:HB2	1:29:A:ILE:HG12	6	0.13
(1,1031)	1:28:A:LYS:HB2	1:29:A:ILE:HG13	6	0.13
(1,1031)	1:28:A:LYS:HB3	1:29:A:ILE:HG12	6	0.13
(1,1031)	1:28:A:LYS:HB3	1:29:A:ILE:HG13	6	0.13
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	9	0.13
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	9	0.13
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	9	0.13
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE1	2	0.13
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE2	2	0.13
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE3	2	0.13
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD1	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD2	4	0.13
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD1	6	0.13
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD2	6	0.13
(1,979)	1:89:A:PHE:HE1	1:128:A:ILE:HB	7	0.13
(1,979)	1:89:A:PHE:HE2	1:128:A:ILE:HB	7	0.13
(1,950)	1:116:A:MET:HE1	1:117:A:ILE:H	9	0.13
(1,950)	1:116:A:MET:HE2	1:117:A:ILE:H	9	0.13
(1,950)	1:116:A:MET:HE3	1:117:A:ILE:H	9	0.13
(1,904)	1:101:A:LYS:HG2	1:147:A:ALA:HB1	7	0.13
(1,904)	1:101:A:LYS:HG2	1:147:A:ALA:HB2	7	0.13
(1,904)	1:101:A:LYS:HG2	1:147:A:ALA:HB3	7	0.13
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	6	0.13
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	6	0.13
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	6	0.13
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	6	0.13
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	6	0.13
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	6	0.13
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	6	0.13
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	6	0.13
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	6	0.13
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG21	5	0.13
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG22	5	0.13
(1,895)	1:38:A:ILE:HB	1:42:A:ILE:HG23	5	0.13
(1,850)	1:141:A:LYS:HA	1:142:A:THR:HG21	3	0.13
(1,850)	1:141:A:LYS:HA	1:142:A:THR:HG22	3	0.13
(1,850)	1:141:A:LYS:HA	1:142:A:THR:HG23	3	0.13
(1,840)	1:113:A:TYR:HE1	1:135:A:VAL:HA	4	0.13
(1,840)	1:113:A:TYR:HE2	1:135:A:VAL:HA	4	0.13
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD11	5	0.13
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD12	5	0.13
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD13	5	0.13
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD11	4	0.13
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD12	4	0.13
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD13	4	0.13
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD11	7	0.13
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD12	7	0.13
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD13	7	0.13
(1,765)	1:150:A:ILE:HG21	1:153:A:ILE:H	9	0.13
(1,765)	1:150:A:ILE:HG22	1:153:A:ILE:H	9	0.13
(1,765)	1:150:A:ILE:HG23	1:153:A:ILE:H	9	0.13
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	9	0.13
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	9	0.13
(1,715)	1:53:A:GLY:H	1:54:A:VAL:HB	9	0.13
(1,677)	1:91:A:LYS:HD2	1:92:A:ALA:H	1	0.13
(1,677)	1:91:A:LYS:HD3	1:92:A:ALA:H	1	0.13
(1,632)	1:154:A:ALA:H	1:157:A:MET:HE1	7	0.13
(1,632)	1:154:A:ALA:H	1:157:A:MET:HE2	7	0.13
(1,632)	1:154:A:ALA:H	1:157:A:MET:HE3	7	0.13
(1,556)	1:24:A:THR:HB	1:25:A:GLY:H	1	0.13
(1,534)	1:178:A:LYS:HA	1:179:A:ALA:H	3	0.13
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG11	8	0.13
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG12	8	0.13
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG13	8	0.13
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE1	10	0.13
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE2	10	0.13
(1,293)	1:111:A:ALA:HB1	1:112:A:MET:HE3	10	0.13
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE1	10	0.13
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE2	10	0.13
(1,293)	1:111:A:ALA:HB2	1:112:A:MET:HE3	10	0.13
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE1	10	0.13
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE2	10	0.13
(1,293)	1:111:A:ALA:HB3	1:112:A:MET:HE3	10	0.13
(1,282)	1:50:A:LYS:HA	1:50:A:LYS:HD2	6	0.13
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE1	4	0.13
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE2	4	0.13
(1,265)	1:35:A:ALA:HB1	1:116:A:MET:HE3	4	0.13
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE1	4	0.13
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE2	4	0.13
(1,265)	1:35:A:ALA:HB2	1:116:A:MET:HE3	4	0.13
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE1	4	0.13
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE2	4	0.13
(1,265)	1:35:A:ALA:HB3	1:116:A:MET:HE3	4	0.13
(1,203)	1:140:A:GLN:HA	1:140:A:GLN:HG3	2	0.13
(1,203)	1:140:A:GLN:HA	1:140:A:GLN:HG3	10	0.13
(1,129)	1:47:A:ALA:HA	1:51:A:LYS:H	6	0.13
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD11	1	0.13
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD12	1	0.13
(1,118)	1:78:A:ALA:H	1:126:A:ILE:HD13	1	0.13
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE1	4	0.13
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE2	4	0.13
(1,100)	1:128:A:ILE:H	1:131:A:MET:HE3	4	0.13
(1,69)	1:88:A:ARG:HD3	1:92:A:ALA:H	6	0.13
(1,1511)	1:177:A:GLU:HA	1:177:A:GLU:HG2	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:177:A:GLU:HA	1:177:A:GLU:HG3	9	0.12
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG11	5	0.12
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG12	5	0.12
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG13	5	0.12
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG21	5	0.12
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG22	5	0.12
(1,1459)	1:161:A:LEU:HG	1:164:A:VAL:HG23	5	0.12
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG12	2	0.12
(1,1438)	1:144:A:ALA:HA	1:153:A:ILE:HG13	2	0.12
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE1	10	0.12
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE2	10	0.12
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE3	10	0.12
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE1	10	0.12
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE2	10	0.12
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE3	10	0.12
(1,1400)	1:128:A:ILE:HG12	1:129:A:GLN:H	8	0.12
(1,1400)	1:128:A:ILE:HG13	1:129:A:GLN:H	8	0.12
(1,1349)	1:116:A:MET:HA	1:119:A:VAL:HG11	2	0.12
(1,1349)	1:116:A:MET:HA	1:119:A:VAL:HG12	2	0.12
(1,1349)	1:116:A:MET:HA	1:119:A:VAL:HG13	2	0.12
(1,1349)	1:116:A:MET:HA	1:119:A:VAL:HG21	2	0.12
(1,1349)	1:116:A:MET:HA	1:119:A:VAL:HG22	2	0.12
(1,1349)	1:116:A:MET:HA	1:119:A:VAL:HG23	2	0.12
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB2	8	0.12
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB3	8	0.12
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB1	2	0.12
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB2	2	0.12
(1,1289)	1:100:A:LEU:HB2	1:108:A:ALA:HB3	2	0.12
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB1	2	0.12
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB2	2	0.12
(1,1289)	1:100:A:LEU:HB3	1:108:A:ALA:HB3	2	0.12
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB2	7	0.12
(1,1288)	1:100:A:LEU:HA	1:103:A:SER:HB3	7	0.12
(1,1239)	1:88:A:ARG:HD2	1:89:A:PHE:H	3	0.12
(1,1239)	1:88:A:ARG:HD3	1:89:A:PHE:H	3	0.12
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB1	9	0.12
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB2	9	0.12
(1,1238)	1:88:A:ARG:HG2	1:92:A:ALA:HB3	9	0.12
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB1	9	0.12
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB2	9	0.12
(1,1238)	1:88:A:ARG:HG3	1:92:A:ALA:HB3	9	0.12
(1,1237)	1:88:A:ARG:HG2	1:92:A:ALA:HA	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:88:A:ARG:HG3	1:92:A:ALA:HA	4	0.12
(1,1166)	1:72:A:PRO:HA	1:175:A:LEU:HD11	8	0.12
(1,1166)	1:72:A:PRO:HA	1:175:A:LEU:HD12	8	0.12
(1,1166)	1:72:A:PRO:HA	1:175:A:LEU:HD13	8	0.12
(1,1166)	1:72:A:PRO:HA	1:175:A:LEU:HD21	8	0.12
(1,1166)	1:72:A:PRO:HA	1:175:A:LEU:HD22	8	0.12
(1,1166)	1:72:A:PRO:HA	1:175:A:LEU:HD23	8	0.12
(1,1160)	1:68:A:ILE:HG12	1:69:A:SER:H	4	0.12
(1,1160)	1:68:A:ILE:HG13	1:69:A:SER:H	4	0.12
(1,1160)	1:68:A:ILE:HG12	1:69:A:SER:H	7	0.12
(1,1160)	1:68:A:ILE:HG13	1:69:A:SER:H	7	0.12
(1,1120)	1:54:A:VAL:HG11	1:75:A:ILE:HG21	9	0.12
(1,1120)	1:54:A:VAL:HG11	1:75:A:ILE:HG22	9	0.12
(1,1120)	1:54:A:VAL:HG11	1:75:A:ILE:HG23	9	0.12
(1,1120)	1:54:A:VAL:HG12	1:75:A:ILE:HG21	9	0.12
(1,1120)	1:54:A:VAL:HG12	1:75:A:ILE:HG22	9	0.12
(1,1120)	1:54:A:VAL:HG12	1:75:A:ILE:HG23	9	0.12
(1,1120)	1:54:A:VAL:HG13	1:75:A:ILE:HG21	9	0.12
(1,1120)	1:54:A:VAL:HG13	1:75:A:ILE:HG22	9	0.12
(1,1120)	1:54:A:VAL:HG13	1:75:A:ILE:HG23	9	0.12
(1,1120)	1:54:A:VAL:HG21	1:75:A:ILE:HG21	9	0.12
(1,1120)	1:54:A:VAL:HG21	1:75:A:ILE:HG22	9	0.12
(1,1120)	1:54:A:VAL:HG21	1:75:A:ILE:HG23	9	0.12
(1,1120)	1:54:A:VAL:HG22	1:75:A:ILE:HG21	9	0.12
(1,1120)	1:54:A:VAL:HG22	1:75:A:ILE:HG22	9	0.12
(1,1120)	1:54:A:VAL:HG22	1:75:A:ILE:HG23	9	0.12
(1,1120)	1:54:A:VAL:HG23	1:75:A:ILE:HG21	9	0.12
(1,1120)	1:54:A:VAL:HG23	1:75:A:ILE:HG22	9	0.12
(1,1120)	1:54:A:VAL:HG23	1:75:A:ILE:HG23	9	0.12
(1,1100)	1:51:A:LYS:H	1:51:A:LYS:HD2	2	0.12
(1,1100)	1:51:A:LYS:H	1:51:A:LYS:HD3	2	0.12
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD1	9	0.12
(1,982)	1:35:A:ALA:HA	1:89:A:PHE:HD2	9	0.12
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE1	9	0.12
(1,975)	1:56:A:PHE:HA	1:59:A:PHE:HE2	9	0.12
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE1	3	0.12
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE2	3	0.12
(1,915)	1:180:A:LYS:HA	1:181:A:THR:HG21	2	0.12
(1,915)	1:180:A:LYS:HA	1:181:A:THR:HG22	2	0.12
(1,915)	1:180:A:LYS:HA	1:181:A:THR:HG23	2	0.12
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB1	4	0.12
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB3	4	0.12
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG21	6	0.12
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG22	6	0.12
(1,880)	1:135:A:VAL:HB	1:153:A:ILE:HG23	6	0.12
(1,873)	1:60:A:THR:HG21	1:61:A:ASN:HB3	7	0.12
(1,873)	1:60:A:THR:HG22	1:61:A:ASN:HB3	7	0.12
(1,873)	1:60:A:THR:HG23	1:61:A:ASN:HB3	7	0.12
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD1	2	0.12
(1,835)	1:45:A:ILE:HG21	1:74:A:PHE:HD2	2	0.12
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD1	2	0.12
(1,835)	1:45:A:ILE:HG22	1:74:A:PHE:HD2	2	0.12
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD1	2	0.12
(1,835)	1:45:A:ILE:HG23	1:74:A:PHE:HD2	2	0.12
(1,830)	1:80:A:ILE:HD11	1:169:A:HIS:HE1	1	0.12
(1,830)	1:80:A:ILE:HD12	1:169:A:HIS:HE1	1	0.12
(1,830)	1:80:A:ILE:HD13	1:169:A:HIS:HE1	1	0.12
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	1	0.12
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	1	0.12
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	1	0.12
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	8	0.12
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	8	0.12
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	8	0.12
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG21	5	0.12
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG22	5	0.12
(1,725)	1:101:A:LYS:H	1:146:A:THR:HG23	5	0.12
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	3	0.12
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	3	0.12
(1,721)	1:126:A:ILE:HG12	1:128:A:ILE:H	10	0.12
(1,721)	1:126:A:ILE:HG13	1:128:A:ILE:H	10	0.12
(1,640)	1:44:A:LYS:HB2	1:48:A:ASN:H	2	0.12
(1,625)	1:140:A:GLN:HB3	1:142:A:THR:H	10	0.12
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	4	0.12
(1,556)	1:24:A:THR:HB	1:25:A:GLY:H	8	0.12
(1,533)	1:49:A:ALA:H	1:50:A:LYS:HA	9	0.12
(1,455)	1:59:A:PHE:H	1:61:A:ASN:H	7	0.12
(1,440)	1:102:A:LYS:H	1:104:A:GLY:H	9	0.12
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD11	9	0.12
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD12	9	0.12
(1,382)	1:92:A:ALA:HA	1:93:A:ILE:HD13	9	0.12
(1,381)	1:115:A:LEU:HA	1:117:A:ILE:HD11	1	0.12
(1,381)	1:115:A:LEU:HA	1:117:A:ILE:HD12	1	0.12
(1,381)	1:115:A:LEU:HA	1:117:A:ILE:HD13	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:45:A:ILE:HD11	1:49:A:ALA:HB1	3	0.12
(1,361)	1:45:A:ILE:HD11	1:49:A:ALA:HB2	3	0.12
(1,361)	1:45:A:ILE:HD11	1:49:A:ALA:HB3	3	0.12
(1,361)	1:45:A:ILE:HD12	1:49:A:ALA:HB1	3	0.12
(1,361)	1:45:A:ILE:HD12	1:49:A:ALA:HB2	3	0.12
(1,361)	1:45:A:ILE:HD12	1:49:A:ALA:HB3	3	0.12
(1,361)	1:45:A:ILE:HD13	1:49:A:ALA:HB1	3	0.12
(1,361)	1:45:A:ILE:HD13	1:49:A:ALA:HB2	3	0.12
(1,361)	1:45:A:ILE:HD13	1:49:A:ALA:HB3	3	0.12
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG21	6	0.12
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG22	6	0.12
(1,313)	1:90:A:VAL:HA	1:93:A:ILE:HG23	6	0.12
(1,268)	1:142:A:THR:HB	1:152:A:ALA:HB1	3	0.12
(1,268)	1:142:A:THR:HB	1:152:A:ALA:HB2	3	0.12
(1,268)	1:142:A:THR:HB	1:152:A:ALA:HB3	3	0.12
(1,257)	1:59:A:PHE:HB2	1:60:A:THR:HA	7	0.12
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG21	6	0.12
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG22	6	0.12
(1,247)	1:59:A:PHE:HB2	1:75:A:ILE:HG23	6	0.12
(1,238)	1:56:A:PHE:HA	1:59:A:PHE:HB3	6	0.12
(1,200)	1:29:A:ILE:HB	1:30:A:ARG:HA	7	0.12
(1,193)	1:85:A:VAL:HA	1:88:A:ARG:HA	5	0.12
(1,179)	1:58:A:ALA:HB1	1:61:A:ASN:HA	2	0.12
(1,179)	1:58:A:ALA:HB2	1:61:A:ASN:HA	2	0.12
(1,179)	1:58:A:ALA:HB3	1:61:A:ASN:HA	2	0.12
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG21	9	0.12
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG22	9	0.12
(1,143)	1:146:A:THR:H	1:150:A:ILE:HG23	9	0.12
(1,127)	1:74:A:PHE:HZ	1:75:A:ILE:HA	2	0.12
(1,122)	1:83:A:ILE:HD11	1:85:A:VAL:H	10	0.12
(1,122)	1:83:A:ILE:HD12	1:85:A:VAL:H	10	0.12
(1,122)	1:83:A:ILE:HD13	1:85:A:VAL:H	10	0.12
(1,60)	1:91:A:LYS:HA	1:93:A:ILE:H	7	0.12
(1,31)	1:131:A:MET:HE1	1:161:A:LEU:H	8	0.12
(1,31)	1:131:A:MET:HE2	1:161:A:LEU:H	8	0.12
(1,31)	1:131:A:MET:HE3	1:161:A:LEU:H	8	0.12
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD2	1	0.11
(1,1435)	1:142:A:THR:HB	1:143:A:PRO:HD3	1	0.11
(1,1429)	1:137:A:GLU:HA	1:140:A:GLN:HG2	9	0.11
(1,1429)	1:137:A:GLU:HA	1:140:A:GLN:HG3	9	0.11
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE1	5	0.11
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1411)	1:130:A:LYS:HG2	1:131:A:MET:HE3	5	0.11
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE1	5	0.11
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE2	5	0.11
(1,1411)	1:130:A:LYS:HG3	1:131:A:MET:HE3	5	0.11
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD11	8	0.11
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD12	8	0.11
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD13	8	0.11
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD11	8	0.11
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD12	8	0.11
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD13	8	0.11
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD11	10	0.11
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD12	10	0.11
(1,1395)	1:127:A:GLY:HA2	1:128:A:ILE:HD13	10	0.11
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD11	10	0.11
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD12	10	0.11
(1,1395)	1:127:A:GLY:HA3	1:128:A:ILE:HD13	10	0.11
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG2	5	0.11
(1,1378)	1:123:A:LEU:HD11	1:129:A:GLN:HG3	5	0.11
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG2	5	0.11
(1,1378)	1:123:A:LEU:HD12	1:129:A:GLN:HG3	5	0.11
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG2	5	0.11
(1,1378)	1:123:A:LEU:HD13	1:129:A:GLN:HG3	5	0.11
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG2	5	0.11
(1,1378)	1:123:A:LEU:HD21	1:129:A:GLN:HG3	5	0.11
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG2	5	0.11
(1,1378)	1:123:A:LEU:HD22	1:129:A:GLN:HG3	5	0.11
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG2	5	0.11
(1,1378)	1:123:A:LEU:HD23	1:129:A:GLN:HG3	5	0.11
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB2	10	0.11
(1,1344)	1:115:A:LEU:HB2	1:118:A:ASP:HB3	10	0.11
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB2	10	0.11
(1,1343)	1:115:A:LEU:HB3	1:118:A:ASP:HB3	10	0.11
(1,1325)	1:106:A:SER:HB2	1:145:A:THR:HG21	1	0.11
(1,1325)	1:106:A:SER:HB2	1:145:A:THR:HG22	1	0.11
(1,1325)	1:106:A:SER:HB2	1:145:A:THR:HG23	1	0.11
(1,1325)	1:106:A:SER:HB3	1:145:A:THR:HG21	1	0.11
(1,1325)	1:106:A:SER:HB3	1:145:A:THR:HG22	1	0.11
(1,1325)	1:106:A:SER:HB3	1:145:A:THR:HG23	1	0.11
(1,1242)	1:89:A:PHE:HB2	1:128:A:ILE:HG21	4	0.11
(1,1242)	1:89:A:PHE:HB2	1:128:A:ILE:HG22	4	0.11
(1,1242)	1:89:A:PHE:HB2	1:128:A:ILE:HG23	4	0.11
(1,1242)	1:89:A:PHE:HB3	1:128:A:ILE:HG21	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1242)	1:89:A:PHE:HB3	1:128:A:ILE:HG22	4	0.11
(1,1242)	1:89:A:PHE:HB3	1:128:A:ILE:HG23	4	0.11
(1,1239)	1:88:A:ARG:HD2	1:89:A:PHE:H	7	0.11
(1,1239)	1:88:A:ARG:HD3	1:89:A:PHE:H	7	0.11
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD11	2	0.11
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD12	2	0.11
(1,1223)	1:85:A:VAL:HG11	1:126:A:ILE:HD13	2	0.11
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD11	2	0.11
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD12	2	0.11
(1,1223)	1:85:A:VAL:HG12	1:126:A:ILE:HD13	2	0.11
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD11	2	0.11
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD12	2	0.11
(1,1223)	1:85:A:VAL:HG13	1:126:A:ILE:HD13	2	0.11
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD11	2	0.11
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD12	2	0.11
(1,1223)	1:85:A:VAL:HG21	1:126:A:ILE:HD13	2	0.11
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD11	2	0.11
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD12	2	0.11
(1,1223)	1:85:A:VAL:HG22	1:126:A:ILE:HD13	2	0.11
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD11	2	0.11
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD12	2	0.11
(1,1223)	1:85:A:VAL:HG23	1:126:A:ILE:HD13	2	0.11
(1,1211)	1:84:A:GLN:HA	1:84:A:GLN:HG2	3	0.11
(1,1211)	1:84:A:GLN:HA	1:84:A:GLN:HG3	3	0.11
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD11	7	0.11
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD12	7	0.11
(1,1156)	1:67:A:LYS:HG2	1:68:A:ILE:HD13	7	0.11
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD11	7	0.11
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD12	7	0.11
(1,1156)	1:67:A:LYS:HG3	1:68:A:ILE:HD13	7	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB1	3	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB2	3	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB3	3	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB1	3	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB2	3	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB3	3	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB1	5	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB2	5	0.11
(1,1135)	1:57:A:GLU:HG2	1:58:A:ALA:HB3	5	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB1	5	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB2	5	0.11
(1,1135)	1:57:A:GLU:HG3	1:58:A:ALA:HB3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1061)	1:39:A:LYS:HA	1:43:A:ASN:HB2	4	0.11
(1,1061)	1:39:A:LYS:HA	1:43:A:ASN:HB3	4	0.11
(1,1056)	1:38:A:ILE:HG12	1:85:A:VAL:HG11	4	0.11
(1,1056)	1:38:A:ILE:HG12	1:85:A:VAL:HG12	4	0.11
(1,1056)	1:38:A:ILE:HG12	1:85:A:VAL:HG13	4	0.11
(1,1056)	1:38:A:ILE:HG12	1:85:A:VAL:HG21	4	0.11
(1,1056)	1:38:A:ILE:HG12	1:85:A:VAL:HG22	4	0.11
(1,1056)	1:38:A:ILE:HG12	1:85:A:VAL:HG23	4	0.11
(1,1056)	1:38:A:ILE:HG13	1:85:A:VAL:HG11	4	0.11
(1,1056)	1:38:A:ILE:HG13	1:85:A:VAL:HG12	4	0.11
(1,1056)	1:38:A:ILE:HG13	1:85:A:VAL:HG13	4	0.11
(1,1056)	1:38:A:ILE:HG13	1:85:A:VAL:HG21	4	0.11
(1,1056)	1:38:A:ILE:HG13	1:85:A:VAL:HG22	4	0.11
(1,1056)	1:38:A:ILE:HG13	1:85:A:VAL:HG23	4	0.11
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE1	5	0.11
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE2	5	0.11
(1,993)	1:94:A:LYS:HA	1:157:A:MET:HE3	5	0.11
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE1	5	0.11
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE2	5	0.11
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD11	4	0.11
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD12	4	0.11
(1,981)	1:90:A:VAL:H	1:128:A:ILE:HD13	4	0.11
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE1	2	0.11
(1,966)	1:56:A:PHE:HA	1:56:A:PHE:HE2	2	0.11
(1,932)	1:128:A:ILE:HG21	1:131:A:MET:HE1	7	0.11
(1,932)	1:128:A:ILE:HG21	1:131:A:MET:HE2	7	0.11
(1,932)	1:128:A:ILE:HG21	1:131:A:MET:HE3	7	0.11
(1,932)	1:128:A:ILE:HG22	1:131:A:MET:HE1	7	0.11
(1,932)	1:128:A:ILE:HG22	1:131:A:MET:HE2	7	0.11
(1,932)	1:128:A:ILE:HG22	1:131:A:MET:HE3	7	0.11
(1,932)	1:128:A:ILE:HG23	1:131:A:MET:HE1	7	0.11
(1,932)	1:128:A:ILE:HG23	1:131:A:MET:HE2	7	0.11
(1,932)	1:128:A:ILE:HG23	1:131:A:MET:HE3	7	0.11
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG21	9	0.11
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG22	9	0.11
(1,929)	1:86:A:ALA:HA	1:126:A:ILE:HG23	9	0.11
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG21	6	0.11
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG22	6	0.11
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG23	6	0.11
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	2	0.11
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	2	0.11
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	2	0.11
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	2	0.11
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	2	0.11
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	2	0.11
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	2	0.11
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	2	0.11
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG21	4	0.11
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG22	4	0.11
(1,899)	1:97:A:ALA:HB1	1:146:A:THR:HG23	4	0.11
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG21	4	0.11
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG22	4	0.11
(1,899)	1:97:A:ALA:HB2	1:146:A:THR:HG23	4	0.11
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG21	4	0.11
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG22	4	0.11
(1,899)	1:97:A:ALA:HB3	1:146:A:THR:HG23	4	0.11
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE1	10	0.11
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE2	10	0.11
(1,889)	1:100:A:LEU:HG	1:112:A:MET:HE3	10	0.11
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB1	3	0.11
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB2	3	0.11
(1,882)	1:135:A:VAL:HB	1:138:A:ALA:HB3	3	0.11
(1,840)	1:113:A:TYR:HE1	1:135:A:VAL:HA	1	0.11
(1,840)	1:113:A:TYR:HE2	1:135:A:VAL:HA	1	0.11
(1,830)	1:80:A:ILE:HD11	1:169:A:HIS:HE1	3	0.11
(1,830)	1:80:A:ILE:HD12	1:169:A:HIS:HE1	3	0.11
(1,830)	1:80:A:ILE:HD13	1:169:A:HIS:HE1	3	0.11
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD11	9	0.11
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD12	9	0.11
(1,776)	1:89:A:PHE:H	1:128:A:ILE:HD13	9	0.11
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD11	7	0.11
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD12	7	0.11
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD13	7	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD11	2	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD12	2	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD13	2	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD11	3	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD12	3	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD13	3	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD11	9	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD12	9	0.11
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD13	9	0.11
(1,765)	1:150:A:ILE:HG21	1:153:A:ILE:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:150:A:ILE:HG22	1:153:A:ILE:H	5	0.11
(1,765)	1:150:A:ILE:HG23	1:153:A:ILE:H	5	0.11
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	8	0.11
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	8	0.11
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	8	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG21	1	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG22	1	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG23	1	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG21	2	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG22	2	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG23	2	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG21	8	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG22	8	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG23	8	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG21	10	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG22	10	0.11
(1,750)	1:24:A:THR:H	1:24:A:THR:HG23	10	0.11
(1,730)	1:90:A:VAL:HG11	1:160:A:LYS:H	7	0.11
(1,730)	1:90:A:VAL:HG12	1:160:A:LYS:H	7	0.11
(1,730)	1:90:A:VAL:HG13	1:160:A:LYS:H	7	0.11
(1,637)	1:131:A:MET:HE1	1:165:A:ASN:H	1	0.11
(1,637)	1:131:A:MET:HE2	1:165:A:ASN:H	1	0.11
(1,637)	1:131:A:MET:HE3	1:165:A:ASN:H	1	0.11
(1,625)	1:140:A:GLN:HB3	1:142:A:THR:H	2	0.11
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	9	0.11
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	10	0.11
(1,571)	1:158:A:GLU:HA	1:162:A:ASN:H	6	0.11
(1,533)	1:49:A:ALA:H	1:50:A:LYS:HA	4	0.11
(1,530)	1:61:A:ASN:HA	1:62:A:THR:H	4	0.11
(1,455)	1:59:A:PHE:H	1:61:A:ASN:H	8	0.11
(1,440)	1:102:A:LYS:H	1:104:A:GLY:H	3	0.11
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG21	7	0.11
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG22	7	0.11
(1,359)	1:100:A:LEU:HD11	1:146:A:THR:HG23	7	0.11
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG21	7	0.11
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG22	7	0.11
(1,359)	1:100:A:LEU:HD12	1:146:A:THR:HG23	7	0.11
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG21	7	0.11
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG22	7	0.11
(1,359)	1:100:A:LEU:HD13	1:146:A:THR:HG23	7	0.11
(1,296)	1:156:A:ALA:HB1	1:157:A:MET:HE1	7	0.11
(1,296)	1:156:A:ALA:HB1	1:157:A:MET:HE2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:156:A:ALA:HB1	1:157:A:MET:HE3	7	0.11
(1,296)	1:156:A:ALA:HB2	1:157:A:MET:HE1	7	0.11
(1,296)	1:156:A:ALA:HB2	1:157:A:MET:HE2	7	0.11
(1,296)	1:156:A:ALA:HB2	1:157:A:MET:HE3	7	0.11
(1,296)	1:156:A:ALA:HB3	1:157:A:MET:HE1	7	0.11
(1,296)	1:156:A:ALA:HB3	1:157:A:MET:HE2	7	0.11
(1,296)	1:156:A:ALA:HB3	1:157:A:MET:HE3	7	0.11
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE1	3	0.11
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE2	3	0.11
(1,292)	1:100:A:LEU:HB3	1:112:A:MET:HE3	3	0.11
(1,180)	1:58:A:ALA:HB1	1:62:A:THR:HB	3	0.11
(1,180)	1:58:A:ALA:HB2	1:62:A:THR:HB	3	0.11
(1,180)	1:58:A:ALA:HB3	1:62:A:THR:HB	3	0.11
(1,180)	1:58:A:ALA:HB1	1:62:A:THR:HB	5	0.11
(1,180)	1:58:A:ALA:HB2	1:62:A:THR:HB	5	0.11
(1,180)	1:58:A:ALA:HB3	1:62:A:THR:HB	5	0.11
(1,174)	1:50:A:LYS:HA	1:50:A:LYS:HG2	6	0.11
(1,135)	1:140:A:GLN:H	1:140:A:GLN:HG3	1	0.11
(1,60)	1:91:A:LYS:HA	1:93:A:ILE:H	1	0.11
(1,29)	1:102:A:LYS:H	1:102:A:LYS:HG3	9	0.11
(1,15)	1:33:A:SER:H	1:33:A:SER:HA	2	0.11
(1,1517)	1:180:A:LYS:H	1:180:A:LYS:HB2	4	0.1
(1,1517)	1:180:A:LYS:H	1:180:A:LYS:HB3	4	0.1
(1,1515)	1:177:A:GLU:HG2	1:179:A:ALA:H	10	0.1
(1,1515)	1:177:A:GLU:HG3	1:179:A:ALA:H	10	0.1
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG11	1	0.1
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG12	1	0.1
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG13	1	0.1
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG21	1	0.1
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG22	1	0.1
(1,1225)	1:86:A:ALA:HB1	1:164:A:VAL:HG23	1	0.1
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG11	1	0.1
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG12	1	0.1
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG13	1	0.1
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG21	1	0.1
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG22	1	0.1
(1,1225)	1:86:A:ALA:HB2	1:164:A:VAL:HG23	1	0.1
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG11	1	0.1
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG12	1	0.1
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG13	1	0.1
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG21	1	0.1
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG22	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:86:A:ALA:HB3	1:164:A:VAL:HG23	1	0.1
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD11	9	0.1
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD12	9	0.1
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD13	9	0.1
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD21	9	0.1
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD22	9	0.1
(1,1172)	1:73:A:GLU:H	1:172:A:LEU:HD23	9	0.1
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB2	6	0.1
(1,1024)	1:27:A:THR:HG21	1:28:A:LYS:HB3	6	0.1
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB2	6	0.1
(1,1024)	1:27:A:THR:HG22	1:28:A:LYS:HB3	6	0.1
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB2	6	0.1
(1,1024)	1:27:A:THR:HG23	1:28:A:LYS:HB3	6	0.1
(1,1023)	1:27:A:THR:H	1:28:A:LYS:HG2	7	0.1
(1,1023)	1:27:A:THR:H	1:28:A:LYS:HG3	7	0.1
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD11	8	0.1
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD12	8	0.1
(1,1009)	1:113:A:TYR:HB3	1:150:A:ILE:HD13	8	0.1
(1,1004)	1:45:A:ILE:HD11	1:74:A:PHE:HD1	5	0.1
(1,1004)	1:45:A:ILE:HD11	1:74:A:PHE:HD2	5	0.1
(1,1004)	1:45:A:ILE:HD12	1:74:A:PHE:HD1	5	0.1
(1,1004)	1:45:A:ILE:HD12	1:74:A:PHE:HD2	5	0.1
(1,1004)	1:45:A:ILE:HD13	1:74:A:PHE:HD1	5	0.1
(1,1004)	1:45:A:ILE:HD13	1:74:A:PHE:HD2	5	0.1
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE1	9	0.1
(1,991)	1:86:A:ALA:HA	1:89:A:PHE:HE2	9	0.1
(1,979)	1:89:A:PHE:HE1	1:128:A:ILE:HB	2	0.1
(1,979)	1:89:A:PHE:HE2	1:128:A:ILE:HB	2	0.1
(1,979)	1:89:A:PHE:HE1	1:128:A:ILE:HB	6	0.1
(1,979)	1:89:A:PHE:HE2	1:128:A:ILE:HB	6	0.1
(1,950)	1:116:A:MET:HE1	1:117:A:ILE:H	8	0.1
(1,950)	1:116:A:MET:HE2	1:117:A:ILE:H	8	0.1
(1,950)	1:116:A:MET:HE3	1:117:A:ILE:H	8	0.1
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG21	8	0.1
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG22	8	0.1
(1,925)	1:28:A:LYS:HA	1:29:A:ILE:HG23	8	0.1
(1,886)	1:64:A:THR:HG21	1:67:A:LYS:HB3	5	0.1
(1,886)	1:64:A:THR:HG22	1:67:A:LYS:HB3	5	0.1
(1,886)	1:64:A:THR:HG23	1:67:A:LYS:HB3	5	0.1
(1,885)	1:90:A:VAL:HG21	1:157:A:MET:HE1	8	0.1
(1,885)	1:90:A:VAL:HG21	1:157:A:MET:HE2	8	0.1
(1,885)	1:90:A:VAL:HG21	1:157:A:MET:HE3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:90:A:VAL:HG22	1:157:A:MET:HE1	8	0.1
(1,885)	1:90:A:VAL:HG22	1:157:A:MET:HE2	8	0.1
(1,885)	1:90:A:VAL:HG22	1:157:A:MET:HE3	8	0.1
(1,885)	1:90:A:VAL:HG23	1:157:A:MET:HE1	8	0.1
(1,885)	1:90:A:VAL:HG23	1:157:A:MET:HE2	8	0.1
(1,885)	1:90:A:VAL:HG23	1:157:A:MET:HE3	8	0.1
(1,871)	1:90:A:VAL:HG11	1:91:A:LYS:HE2	5	0.1
(1,871)	1:90:A:VAL:HG11	1:91:A:LYS:HE3	5	0.1
(1,871)	1:90:A:VAL:HG12	1:91:A:LYS:HE2	5	0.1
(1,871)	1:90:A:VAL:HG12	1:91:A:LYS:HE3	5	0.1
(1,871)	1:90:A:VAL:HG13	1:91:A:LYS:HE2	5	0.1
(1,871)	1:90:A:VAL:HG13	1:91:A:LYS:HE3	5	0.1
(1,838)	1:169:A:HIS:HD2	1:172:A:LEU:HD11	3	0.1
(1,838)	1:169:A:HIS:HD2	1:172:A:LEU:HD12	3	0.1
(1,838)	1:169:A:HIS:HD2	1:172:A:LEU:HD13	3	0.1
(1,830)	1:80:A:ILE:HD11	1:169:A:HIS:HE1	9	0.1
(1,830)	1:80:A:ILE:HD12	1:169:A:HIS:HE1	9	0.1
(1,830)	1:80:A:ILE:HD13	1:169:A:HIS:HE1	9	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	2	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	2	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	2	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	3	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	3	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	3	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD11	9	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD12	9	0.1
(1,809)	1:126:A:ILE:H	1:126:A:ILE:HD13	9	0.1
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD11	8	0.1
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD12	8	0.1
(1,768)	1:171:A:ALA:H	1:172:A:LEU:HD13	8	0.1
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD11	1	0.1
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD12	1	0.1
(1,767)	1:128:A:ILE:H	1:128:A:ILE:HD13	1	0.1
(1,758)	1:145:A:THR:HG21	1:146:A:THR:H	5	0.1
(1,758)	1:145:A:THR:HG22	1:146:A:THR:H	5	0.1
(1,758)	1:145:A:THR:HG23	1:146:A:THR:H	5	0.1
(1,625)	1:140:A:GLN:HB3	1:142:A:THR:H	4	0.1
(1,597)	1:131:A:MET:HG2	1:132:A:THR:H	7	0.1
(1,597)	1:131:A:MET:HG2	1:132:A:THR:H	8	0.1
(1,583)	1:152:A:ALA:H	1:153:A:ILE:HA	6	0.1
(1,533)	1:49:A:ALA:H	1:50:A:LYS:HA	3	0.1
(1,532)	1:181:A:THR:HA	1:182:A:ALA:H	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:88:A:ARG:H	1:88:A:ARG:HG2	5	0.1
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG21	1	0.1
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG22	1	0.1
(1,377)	1:59:A:PHE:HA	1:75:A:ILE:HG23	1	0.1
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD11	6	0.1
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD12	6	0.1
(1,336)	1:28:A:LYS:HA	1:29:A:ILE:HD13	6	0.1
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG11	9	0.1
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG12	9	0.1
(1,333)	1:87:A:GLU:HA	1:90:A:VAL:HG13	9	0.1
(1,207)	1:90:A:VAL:HG21	1:154:A:ALA:HA	5	0.1
(1,207)	1:90:A:VAL:HG22	1:154:A:ALA:HA	5	0.1
(1,207)	1:90:A:VAL:HG23	1:154:A:ALA:HA	5	0.1
(1,203)	1:140:A:GLN:HA	1:140:A:GLN:HG3	8	0.1
(1,122)	1:83:A:ILE:HD11	1:85:A:VAL:H	1	0.1
(1,122)	1:83:A:ILE:HD12	1:85:A:VAL:H	1	0.1
(1,122)	1:83:A:ILE:HD13	1:85:A:VAL:H	1	0.1
(1,60)	1:91:A:LYS:HA	1:93:A:ILE:H	3	0.1
(1,24)	1:95:A:GLU:H	1:95:A:GLU:HG2	6	0.1

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

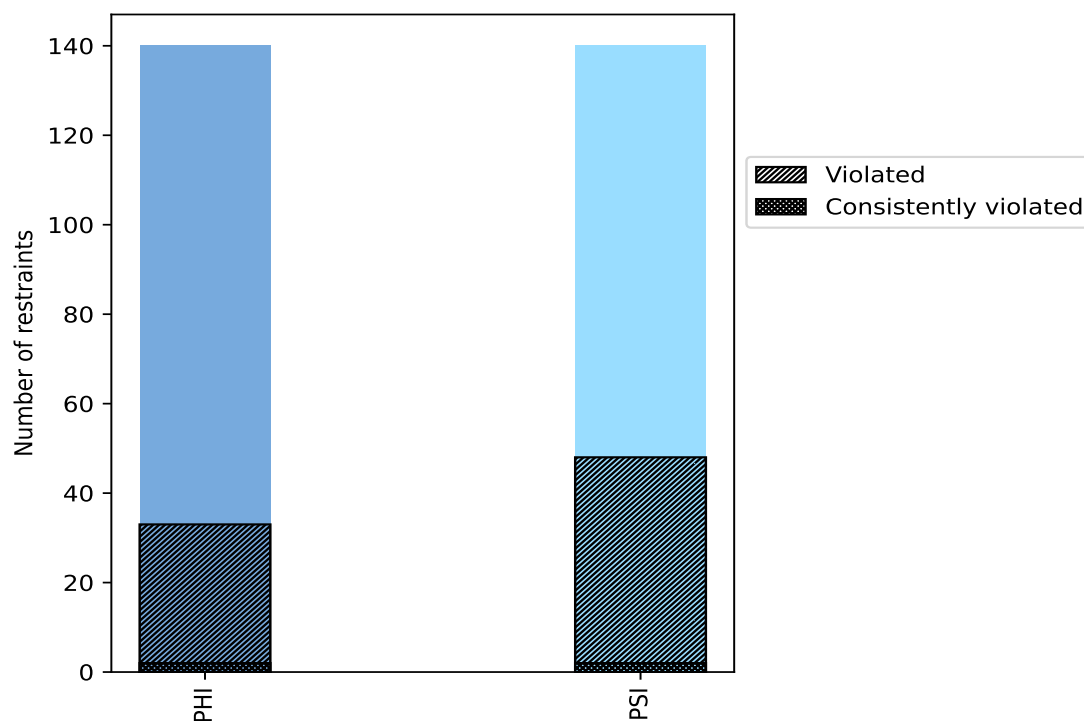
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <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	140	50.0	33	23.6	11.8	2	1.4	0.7
PSI	140	50.0	48	34.3	17.1	2	1.4	0.7
Total	280	100.0	81	28.9	28.9	4	1.4	1.4

<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](#)



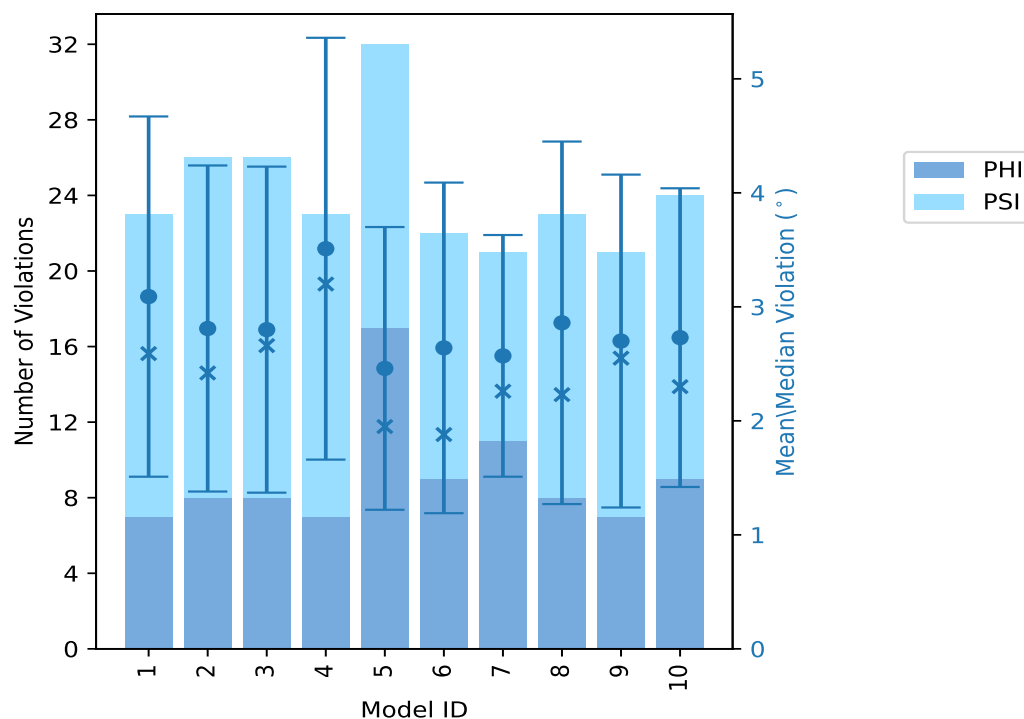
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	16	23	3.09	7.47	1.58	2.59
2	8	18	26	2.81	7.06	1.43	2.42
3	8	18	26	2.8	6.06	1.43	2.66
4	7	16	23	3.51	8.69	1.85	3.2
5	17	15	32	2.46	5.89	1.24	1.95
6	9	13	22	2.64	6.31	1.45	1.88
7	11	10	21	2.57	4.74	1.06	2.26
8	8	15	23	2.86	7.72	1.59	2.23
9	7	14	21	2.7	7.08	1.46	2.55
10	9	15	24	2.73	5.2	1.31	2.3

### 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

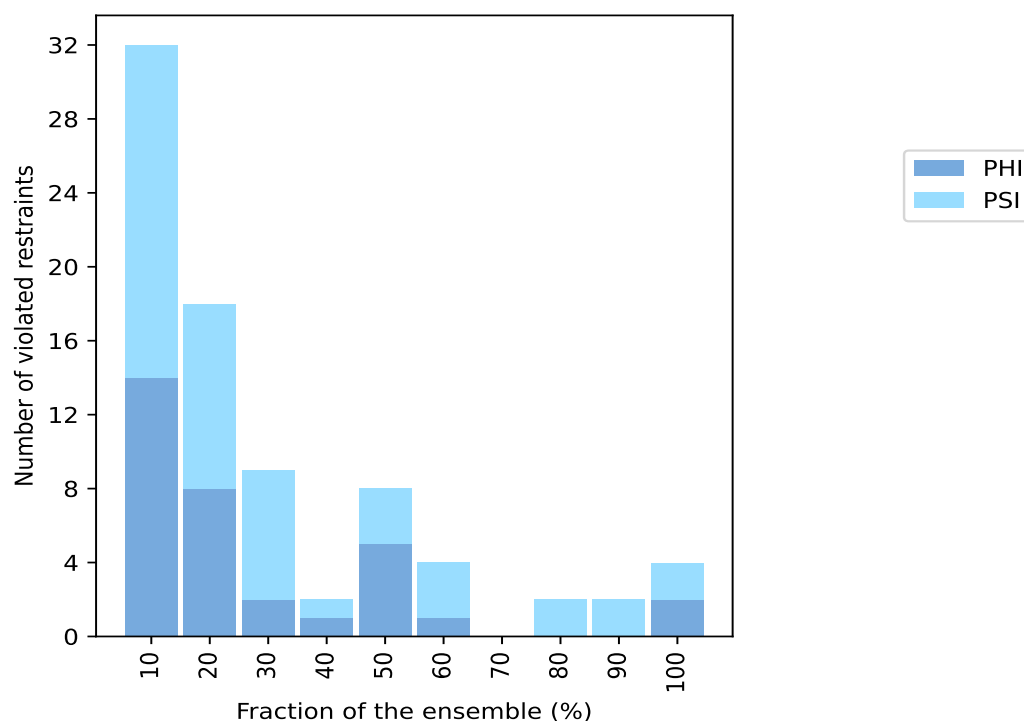
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>	%
14	18	32	1	10.0
8	10	18	2	20.0
2	7	9	3	30.0
1	1	2	4	40.0
5	3	8	5	50.0
1	3	4	6	60.0
0	0	0	7	70.0
0	2	2	8	80.0
0	2	2	9	90.0
2	2	4	10	100.0

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

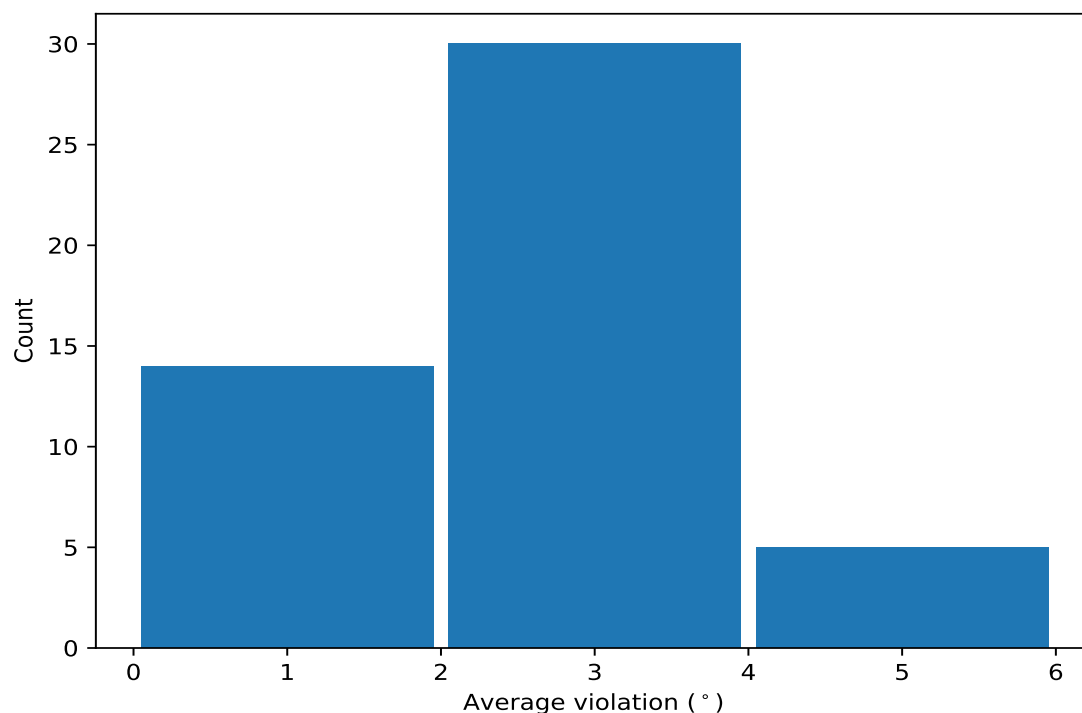
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	10	3.95	2.35	3.34
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	10	3.81	0.9	3.63
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	10	3.46	0.82	3.62
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	10	2.23	0.91	2.05
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	9	3.11	1.26	3.93
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	9	2.57	0.87	2.5
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	8	3.96	1.62	3.45
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	8	2.05	0.66	2.0
(1,116)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:PHE:N	6	5.48	1.86	5.72
(1,216)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:ASP:N	6	3.27	0.91	2.84
(1,6)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:THR:N	6	1.98	0.75	1.81
(1,95)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	6	1.97	0.87	1.84
(1,118)	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	1:90:A:VAL:N	5	4.3	1.19	4.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,114)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ARG:N	5	3.82	1.67	3.04
(1,103)	1:81:A:LYS:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	5	3.52	1.4	3.28
(1,115)	1:87:A:GLU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	5	3.49	1.07	3.28
(1,51)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	5	2.83	1.17	2.87
(1,196)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:VAL:N	5	2.19	1.41	1.44
(1,217)	1:147:A:ALA:C	1:148:A:ASP:N	1:148:A:ASP:CA	1:148:A:ASP:C	5	1.86	0.43	1.97
(1,67)	1:59:A:PHE:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	5	1.8	0.45	1.92
(1,73)	1:62:A:THR:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	4	1.94	0.62	1.96
(1,70)	1:61:A:ASN:N	1:61:A:ASN:CA	1:61:A:ASN:C	1:62:A:THR:N	4	1.74	0.11	1.74
(1,268)	1:174:A:ASN:N	1:174:A:ASN:CA	1:174:A:ASN:C	1:175:A:LEU:N	3	4.55	1.84	4.39
(1,142)	1:102:A:LYS:N	1:102:A:LYS:CA	1:102:A:LYS:C	1:103:A:SER:N	3	4.2	1.0	4.76
(1,78)	1:65:A:GLY:N	1:65:A:GLY:CA	1:65:A:GLY:C	1:66:A:SER:N	3	3.79	1.97	4.63
(1,102)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:ALA:N	3	3.34	0.58	3.74
(1,252)	1:166:A:LYS:N	1:166:A:LYS:CA	1:166:A:LYS:C	1:167:A:LYS:N	3	3.08	0.48	3.14
(1,270)	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	1:176:A:LYS:N	3	2.6	0.92	2.02
(1,133)	1:96:A:GLU:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	3	2.55	0.67	3.0
(1,170)	1:118:A:ASP:C	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	3	2.08	0.44	1.93
(1,64)	1:58:A:ALA:N	1:58:A:ALA:CA	1:58:A:ALA:C	1:59:A:PHE:N	3	1.65	0.4	1.49
(1,141)	1:100:A:LEU:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	2	4.3	1.59	4.3
(1,90)	1:74:A:PHE:N	1:74:A:PHE:CA	1:74:A:PHE:C	1:75:A:ILE:N	2	3.38	1.4	3.38
(1,146)	1:106:A:SER:N	1:106:A:SER:CA	1:106:A:SER:C	1:107:A:GLY:N	2	3.16	1.66	3.16
(1,20)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:GLU:N	2	3.1	1.68	3.1
(1,211)	1:143:A:PRO:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	2	2.89	0.71	2.89
(1,44)	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	1:49:A:ALA:N	2	2.72	0.98	2.72
(1,22)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:ILE:N	2	2.7	0.99	2.7
(1,207)	1:139:A:ALA:C	1:140:A:GLN:N	1:140:A:GLN:CA	1:140:A:GLN:C	2	2.42	1.04	2.42
(1,4)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	2	2.41	0.57	2.41
(1,83)	1:67:A:LYS:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	2	2.27	0.45	2.27
(1,266)	1:173:A:LYS:N	1:173:A:LYS:CA	1:173:A:LYS:C	1:174:A:ASN:N	2	2.22	0.19	2.22
(1,143)	1:102:A:LYS:C	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	2	1.96	0.7	1.96
(1,85)	1:68:A:ILE:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	2	1.93	0.86	1.93
(1,120)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:LYS:N	2	1.86	0.01	1.86
(1,79)	1:65:A:GLY:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	2	1.65	0.11	1.65
(1,75)	1:63:A:GLN:C	1:64:A:THR:N	1:64:A:THR:CA	1:64:A:THR:C	2	1.5	0.0	1.5
(1,188)	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	1:131:A:MET:N	2	1.32	0.06	1.32
(1,220)	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	1:151:A:ILE:N	2	1.31	0.26	1.31

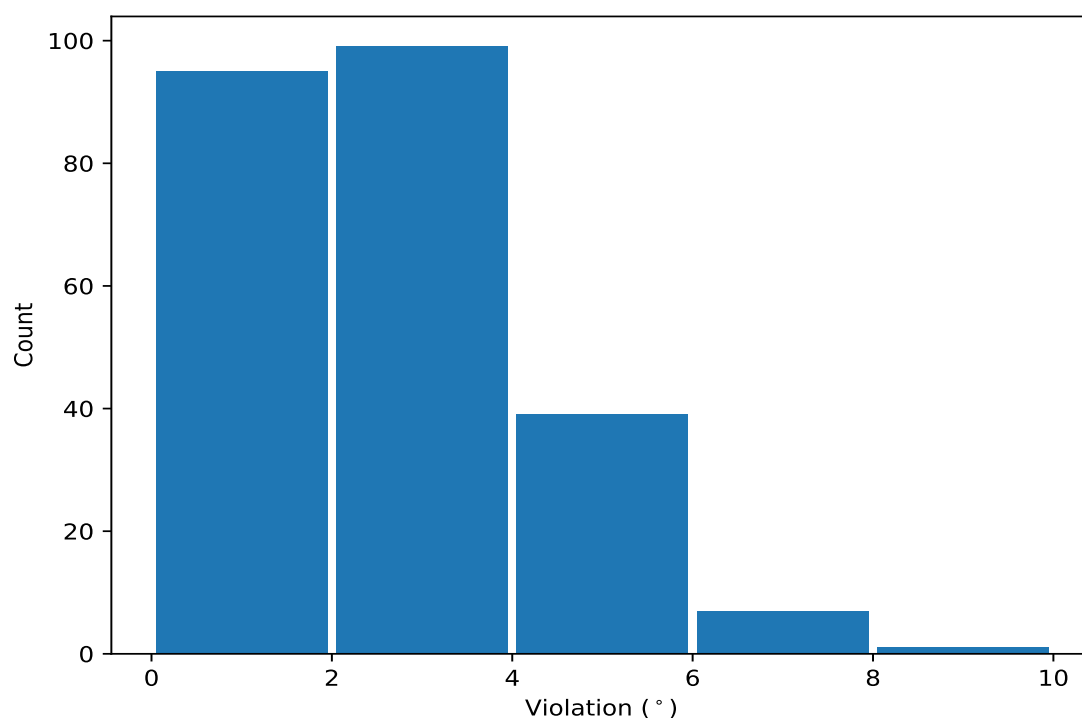
<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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





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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	4	8.69
(1,116)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:PHE:N	8	7.72
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	1	7.47
(1,116)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:PHE:N	9	7.08
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	2	7.06
(1,268)	1:174:A:ASN:N	1:174:A:ASN:CA	1:174:A:ASN:C	1:175:A:LEU:N	4	6.88
(1,116)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:PHE:N	6	6.31
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	3	6.06
(1,118)	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	1:90:A:VAL:N	3	5.99
(1,141)	1:100:A:LEU:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	5	5.89
(1,114)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ARG:N	4	5.85
(1,78)	1:65:A:GLY:N	1:65:A:GLY:CA	1:65:A:GLY:C	1:66:A:SER:N	9	5.68
(1,114)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ARG:N	1	5.66
(1,164)	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	1:116:A:MET:N	4	5.38
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	4	5.36
(1,103)	1:81:A:LYS:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	8	5.21
(1,216)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:ASP:N	10	5.2
(1,116)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:PHE:N	5	5.12
(1,103)	1:81:A:LYS:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	5	5.06
(1,142)	1:102:A:LYS:N	1:102:A:LYS:CA	1:102:A:LYS:C	1:103:A:SER:N	10	5.04
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	3	5.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	1	4.99
(1,196)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:VAL:N	2	4.98
(1,115)	1:87:A:GLU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	8	4.88
(1,118)	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	1:90:A:VAL:N	2	4.85
(1,146)	1:106:A:SER:N	1:106:A:SER:CA	1:106:A:SER:C	1:107:A:GLY:N	1	4.82
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	2	4.8
(1,90)	1:74:A:PHE:N	1:74:A:PHE:CA	1:74:A:PHE:C	1:75:A:ILE:N	2	4.78
(1,20)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:GLU:N	1	4.78
(1,142)	1:102:A:LYS:N	1:102:A:LYS:CA	1:102:A:LYS:C	1:103:A:SER:N	6	4.76
(1,118)	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	1:90:A:VAL:N	7	4.74
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	10	4.67
(1,78)	1:65:A:GLY:N	1:65:A:GLY:CA	1:65:A:GLY:C	1:66:A:SER:N	3	4.63
(1,116)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:PHE:N	10	4.61
(1,51)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	7	4.59
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	10	4.4
(1,268)	1:174:A:ASN:N	1:174:A:ASN:CA	1:174:A:ASN:C	1:175:A:LEU:N	7	4.39
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	1	4.39
(1,115)	1:87:A:GLU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	6	4.35
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	4	4.34
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	8	4.27
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	8	4.24
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	6	4.17
(1,132)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:ALA:N	6	4.07
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	6	4.06
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	1	4.03
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	8	4.02
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	4	3.94
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	5	3.93
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	2	3.91
(1,270)	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	1:176:A:LYS:N	9	3.9
(1,102)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:ALA:N	3	3.76
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	3	3.74
(1,102)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:ALA:N	10	3.74
(1,95)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	3	3.74
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	7	3.72
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	6	3.71
(1,44)	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	1:49:A:ALA:N	3	3.7
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	6	3.69
(1,22)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:ILE:N	10	3.68
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	5	3.66
(1,252)	1:166:A:LYS:N	1:166:A:LYS:CA	1:166:A:LYS:C	1:167:A:LYS:N	8	3.63
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	8	3.63
(1,110)	1:85:A:VAL:N	1:85:A:VAL:CA	1:85:A:VAL:C	1:86:A:ALA:N	4	3.63
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	7	3.61
(1,211)	1:143:A:PRO:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	10	3.6
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	9	3.55
(1,230)	1:155:A:GLN:N	1:155:A:GLN:CA	1:155:A:GLN:C	1:156:A:ALA:N	5	3.54
(1,216)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:ASP:N	4	3.48
(1,207)	1:139:A:ALA:C	1:140:A:GLN:N	1:140:A:GLN:CA	1:140:A:GLN:C	1	3.46
(1,6)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:THR:N	4	3.45
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	2	3.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	4	3.34
(1,51)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	5	3.34
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	5	3.31
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	10	3.3
(1,115)	1:87:A:GLU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	5	3.28
(1,103)	1:81:A:LYS:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	3	3.28
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	5	3.21
(1,118)	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	1:90:A:VAL:N	4	3.2
(1,115)	1:87:A:GLU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	9	3.16
(1,252)	1:166:A:LYS:N	1:166:A:LYS:CA	1:166:A:LYS:C	1:167:A:LYS:N	3	3.14
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	9	3.08
(1,8)	1:27:A:THR:N	1:27:A:THR:CA	1:27:A:THR:C	1:28:A:LYS:N	2	3.08
(1,133)	1:96:A:GLU:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	4	3.06
(1,114)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ARG:N	3	3.04
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	4	3.01
(1,133)	1:96:A:GLU:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	9	3.0
(1,114)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ARG:N	7	2.98
(1,4)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	9	2.97
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	3	2.95
(1,216)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:ASP:N	9	2.94
(1,51)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	2	2.87
(1,5)	1:25:A:GLY:C	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	5	2.87
(1,253)	1:166:A:LYS:C	1:167:A:LYS:N	1:167:A:LYS:CA	1:167:A:LYS:C	1	2.86
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	8	2.84
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	7	2.83
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	9	2.83
(1,142)	1:102:A:LYS:N	1:102:A:LYS:CA	1:102:A:LYS:C	1:103:A:SER:N	1	2.8
(1,212)	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	1:145:A:THR:N	10	2.79
(1,85)	1:68:A:ILE:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	2	2.79
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	4	2.77
(1,216)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:ASP:N	8	2.74
(1,118)	1:89:A:PHE:N	1:89:A:PHE:CA	1:89:A:PHE:C	1:90:A:VAL:N	1	2.73
(1,83)	1:67:A:LYS:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	2	2.72
(1,141)	1:100:A:LEU:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	10	2.7
(1,73)	1:62:A:THR:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	7	2.69
(1,170)	1:118:A:ASP:C	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	6	2.68
(1,216)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:ASP:N	3	2.67
(1,143)	1:102:A:LYS:C	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	5	2.66
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	3	2.65
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	4	2.64
(1,216)	1:147:A:ALA:N	1:147:A:ALA:CA	1:147:A:ALA:C	1:148:A:ASP:N	7	2.6
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	1	2.59
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	1	2.56
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	9	2.55
(1,217)	1:147:A:ALA:C	1:148:A:ASP:N	1:148:A:ASP:CA	1:148:A:ASP:C	4	2.54
(1,102)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:ALA:N	1	2.53
(1,67)	1:59:A:PHE:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	9	2.51
(1,192)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:GLY:N	2	2.5
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	10	2.5
(1,252)	1:166:A:LYS:N	1:166:A:LYS:CA	1:166:A:LYS:C	1:167:A:LYS:N	2	2.47
(1,266)	1:173:A:LYS:N	1:173:A:LYS:CA	1:173:A:LYS:C	1:174:A:ASN:N	8	2.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	7	2.4
(1,73)	1:62:A:THR:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	2	2.38
(1,268)	1:174:A:ASN:N	1:174:A:ASN:CA	1:174:A:ASN:C	1:175:A:LEU:N	5	2.37
(1,51)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	6	2.35
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	7	2.26
(1,84)	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	1:69:A:SER:N	2	2.25
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	8	2.23
(1,6)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:THR:N	8	2.22
(1,260)	1:170:A:ASP:N	1:170:A:ASP:CA	1:170:A:ASP:C	1:171:A:ALA:N	8	2.2
(1,64)	1:58:A:ALA:N	1:58:A:ALA:CA	1:58:A:ALA:C	1:59:A:PHE:N	1	2.2
(1,211)	1:143:A:PRO:C	1:144:A:ALA:N	1:144:A:ALA:CA	1:144:A:ALA:C	5	2.18
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	7	2.17
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	1	2.16
(1,6)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:THR:N	10	2.09
(1,103)	1:81:A:LYS:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	10	2.08
(1,95)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	5	2.08
(1,116)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:PHE:N	7	2.07
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	2	2.06
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	3	2.04
(1,266)	1:173:A:LYS:N	1:173:A:LYS:CA	1:173:A:LYS:C	1:174:A:ASN:N	2	2.03
(1,270)	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	1:176:A:LYS:N	2	2.02
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	5	2.02
(1,217)	1:147:A:ALA:C	1:148:A:ASP:N	1:148:A:ASP:CA	1:148:A:ASP:C	7	2.0
(1,90)	1:74:A:PHE:N	1:74:A:PHE:CA	1:74:A:PHE:C	1:75:A:ILE:N	4	1.98
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	2	1.98
(1,217)	1:147:A:ALA:C	1:148:A:ASP:N	1:148:A:ASP:CA	1:148:A:ASP:C	3	1.97
(1,103)	1:81:A:LYS:C	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	7	1.96
(1,95)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	10	1.96
(1,193)	1:132:A:THR:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	8	1.94
(1,176)	1:122:A:PRO:C	1:123:A:LEU:N	1:123:A:LEU:CA	1:123:A:LEU:C	9	1.93
(1,170)	1:118:A:ASP:C	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	8	1.93
(1,67)	1:59:A:PHE:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	7	1.93
(1,67)	1:59:A:PHE:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	1	1.92
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	1	1.9
(1,70)	1:61:A:ASN:N	1:61:A:ASN:CA	1:61:A:ASN:C	1:62:A:THR:N	6	1.89
(1,270)	1:175:A:LEU:N	1:175:A:LEU:CA	1:175:A:LEU:C	1:176:A:LYS:N	5	1.88
(1,120)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:LYS:N	5	1.88
(1,196)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:VAL:N	6	1.86
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	5	1.86
(1,120)	1:90:A:VAL:N	1:90:A:VAL:CA	1:90:A:VAL:C	1:91:A:LYS:N	6	1.85
(1,24)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:LYS:N	3	1.85
(1,4)	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	1:25:A:GLY:N	5	1.84
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	2	1.83
(1,83)	1:67:A:LYS:C	1:68:A:ILE:N	1:68:A:ILE:CA	1:68:A:ILE:C	7	1.82
(1,70)	1:61:A:ASN:N	1:61:A:ASN:CA	1:61:A:ASN:C	1:62:A:THR:N	10	1.8
(1,115)	1:87:A:GLU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	10	1.78
(1,79)	1:65:A:GLY:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	8	1.76
(1,44)	1:48:A:ASN:N	1:48:A:ASN:CA	1:48:A:ASN:C	1:49:A:ALA:N	7	1.74
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	9	1.73
(1,104)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:ILE:N	4	1.72
(1,95)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	9	1.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:ILE:N	3	1.71
(1,70)	1:61:A:ASN:N	1:61:A:ASN:CA	1:61:A:ASN:C	1:62:A:THR:N	8	1.67
(1,86)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:LYS:N	2	1.64
(1,170)	1:118:A:ASP:C	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	3	1.63
(1,94)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:LYS:N	1	1.63
(1,194)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:THR:N	8	1.61
(1,70)	1:61:A:ASN:N	1:61:A:ASN:CA	1:61:A:ASN:C	1:62:A:THR:N	5	1.61
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	6	1.6
(1,162)	1:114:A:ASP:N	1:114:A:ASP:CA	1:114:A:ASP:C	1:115:A:LEU:N	1	1.6
(1,133)	1:96:A:GLU:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	5	1.6
(1,220)	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	1:151:A:ILE:N	10	1.57
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	10	1.57
(1,114)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ARG:N	10	1.57
(1,63)	1:57:A:GLU:C	1:58:A:ALA:N	1:58:A:ALA:CA	1:58:A:ALA:C	4	1.57
(1,166)	1:116:A:MET:N	1:116:A:MET:CA	1:116:A:MET:C	1:117:A:ILE:N	6	1.55
(1,79)	1:65:A:GLY:C	1:66:A:SER:N	1:66:A:SER:CA	1:66:A:SER:C	3	1.54
(1,73)	1:62:A:THR:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	5	1.53
(1,6)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:THR:N	5	1.53
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	2	1.51
(1,146)	1:106:A:SER:N	1:106:A:SER:CA	1:106:A:SER:C	1:107:A:GLY:N	4	1.51
(1,75)	1:63:A:GLN:C	1:64:A:THR:N	1:64:A:THR:CA	1:64:A:THR:C	5	1.5
(1,75)	1:63:A:GLN:C	1:64:A:THR:N	1:64:A:THR:CA	1:64:A:THR:C	6	1.5
(1,64)	1:58:A:ALA:N	1:58:A:ALA:CA	1:58:A:ALA:C	1:59:A:PHE:N	3	1.49
(1,278)	1:182:A:ALA:N	1:182:A:ALA:CA	1:182:A:ALA:C	1:183:A:THR:N	3	1.48
(1,65)	1:58:A:ALA:C	1:59:A:PHE:N	1:59:A:PHE:CA	1:59:A:PHE:C	1	1.48
(1,196)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:VAL:N	3	1.44
(1,182)	1:125:A:GLU:C	1:126:A:ILE:N	1:126:A:ILE:CA	1:126:A:ILE:C	5	1.44
(1,217)	1:147:A:ALA:C	1:148:A:ASP:N	1:148:A:ASP:CA	1:148:A:ASP:C	9	1.43
(1,20)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:GLU:N	9	1.43
(1,196)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:VAL:N	9	1.41
(1,185)	1:127:A:GLY:N	1:127:A:GLY:CA	1:127:A:GLY:C	1:128:A:ILE:N	6	1.41
(1,67)	1:59:A:PHE:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	6	1.4
(1,233)	1:156:A:ALA:C	1:157:A:MET:N	1:157:A:MET:CA	1:157:A:MET:C	5	1.39
(1,188)	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	1:131:A:MET:N	1	1.39
(1,207)	1:139:A:ALA:C	1:140:A:GLN:N	1:140:A:GLN:CA	1:140:A:GLN:C	2	1.38
(1,6)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:THR:N	6	1.38
(1,217)	1:147:A:ALA:C	1:148:A:ASP:N	1:148:A:ASP:CA	1:148:A:ASP:C	8	1.35
(1,15)	1:31:A:LEU:C	1:32:A:GLU:N	1:32:A:GLU:CA	1:32:A:GLU:C	5	1.34
(1,95)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	2	1.31
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	3	1.3
(1,250)	1:165:A:ASN:N	1:165:A:ASN:CA	1:165:A:ASN:C	1:166:A:LYS:N	10	1.29
(1,3)	1:23:A:LEU:C	1:24:A:THR:N	1:24:A:THR:CA	1:24:A:THR:C	6	1.29
(1,196)	1:134:A:THR:N	1:134:A:THR:CA	1:134:A:THR:C	1:135:A:VAL:N	10	1.27
(1,188)	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	1:131:A:MET:N	2	1.26
(1,64)	1:58:A:ALA:N	1:58:A:ALA:CA	1:58:A:ALA:C	1:59:A:PHE:N	9	1.26
(1,34)	1:43:A:ASN:N	1:43:A:ASN:CA	1:43:A:ASN:C	1:44:A:LYS:N	9	1.26
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	8	1.25
(1,143)	1:102:A:LYS:C	1:103:A:SER:N	1:103:A:SER:CA	1:103:A:SER:C	7	1.25
(1,6)	1:26:A:GLU:N	1:26:A:GLU:CA	1:26:A:GLU:C	1:27:A:THR:N	9	1.23
(1,67)	1:59:A:PHE:C	1:60:A:THR:N	1:60:A:THR:CA	1:60:A:THR:C	4	1.22
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	5	1.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,99)	1:79:A:LYS:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	5	1.21
(1,10)	1:28:A:LYS:N	1:28:A:LYS:CA	1:28:A:LYS:C	1:29:A:ILE:N	5	1.21
(1,73)	1:62:A:THR:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	10	1.16
(1,181)	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	1:126:A:ILE:N	5	1.14
(1,61)	1:56:A:PHE:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	7	1.14
(1,251)	1:165:A:ASN:C	1:166:A:LYS:N	1:166:A:LYS:CA	1:166:A:LYS:C	4	1.12
(1,187)	1:129:A:GLN:C	1:130:A:LYS:N	1:130:A:LYS:CA	1:130:A:LYS:C	6	1.12
(1,267)	1:173:A:LYS:C	1:174:A:ASN:N	1:174:A:ASN:CA	1:174:A:ASN:C	3	1.09
(1,219)	1:149:A:GLY:C	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	10	1.07
(1,85)	1:68:A:ILE:C	1:69:A:SER:N	1:69:A:SER:CA	1:69:A:SER:C	7	1.07
(1,78)	1:65:A:GLY:N	1:65:A:GLY:CA	1:65:A:GLY:C	1:66:A:SER:N	8	1.07
(1,74)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:THR:N	2	1.07
(1,220)	1:150:A:ILE:N	1:150:A:ILE:CA	1:150:A:ILE:C	1:151:A:ILE:N	8	1.04
(1,256)	1:168:A:GLN:N	1:168:A:GLN:CA	1:168:A:GLN:C	1:169:A:HIS:N	3	1.02
(1,95)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	6	1.02
(1,51)	1:51:A:LYS:C	1:52:A:GLU:N	1:52:A:GLU:CA	1:52:A:GLU:C	1	1.01