Full wwPDB NMR Structure Validation Report (i)

Dec 24, 2024 – 11:44 PM EST

PDB ID	:	2MVG
BMRB ID	:	25266
Title	:	Solution structure of decorin binding protein B from Borrelia burgdorferi
Authors	:	Wang, X.; Feng, W.
Deposited on	:	2014-10-03

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

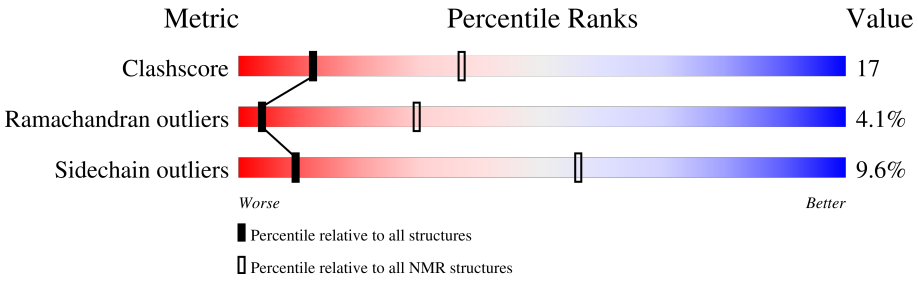
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 84%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	167	54% 19% • 26%

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:32-A:57, A:74-A:170 (123)	0.96	1

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

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

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

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2652 atoms, of which 1376 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	167	Total	C	H	N	O	S	0
			2652	803	1376	222	249	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	SER	-	expression tag	UNP P0CL68

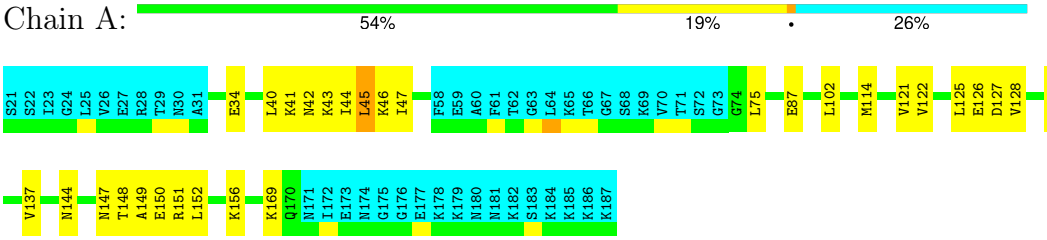
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Decorin-binding protein B

Chain A:



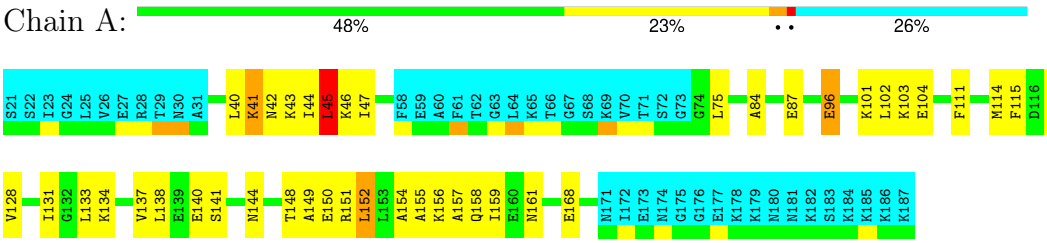
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Decorin-binding protein B

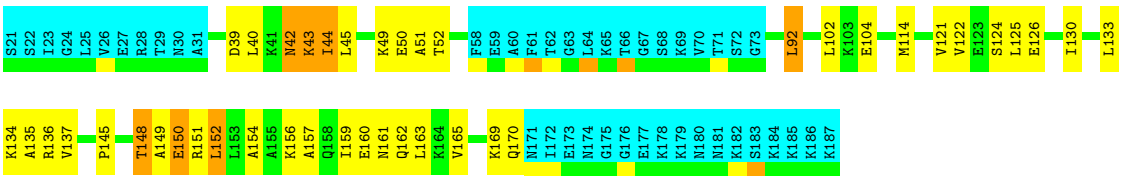
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Decorin-binding protein B

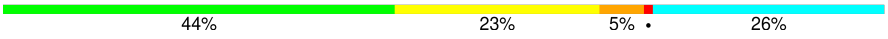
Chain A:

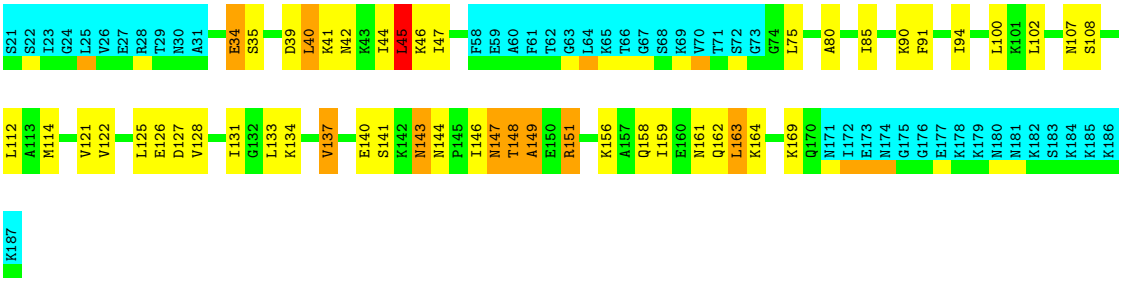


4.2.3 Score per residue for model 3

• Molecule 1: Decorin-binding protein B

Chain A:

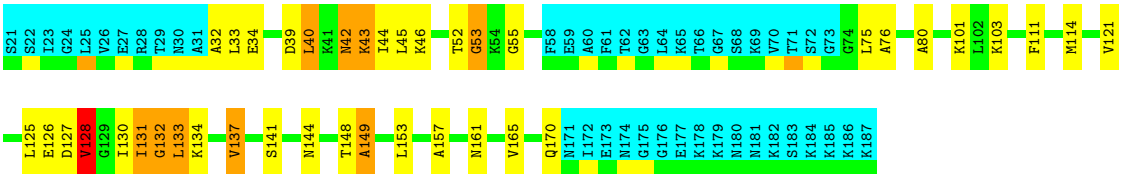




4.2.4 Score per residue for model 4

• Molecule 1: Decorin-binding protein B

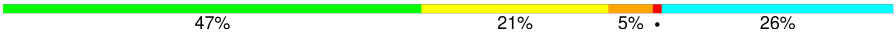
Chain A:

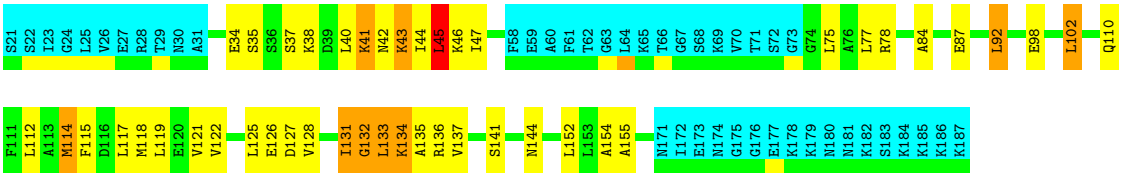


4.2.5 Score per residue for model 5

• Molecule 1: Decorin-binding protein B

Chain A:

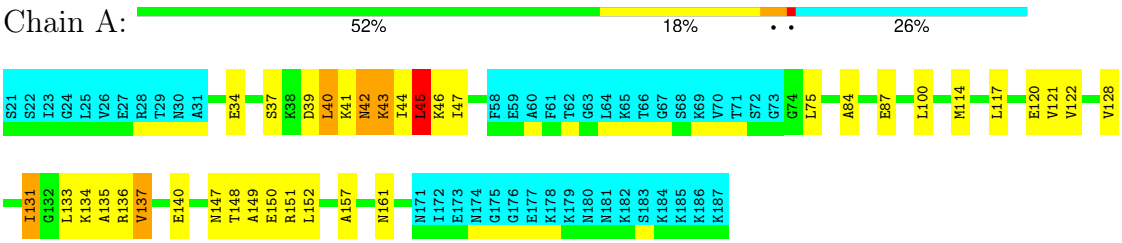




4.2.6 Score per residue for model 6

• Molecule 1: Decorin-binding protein B

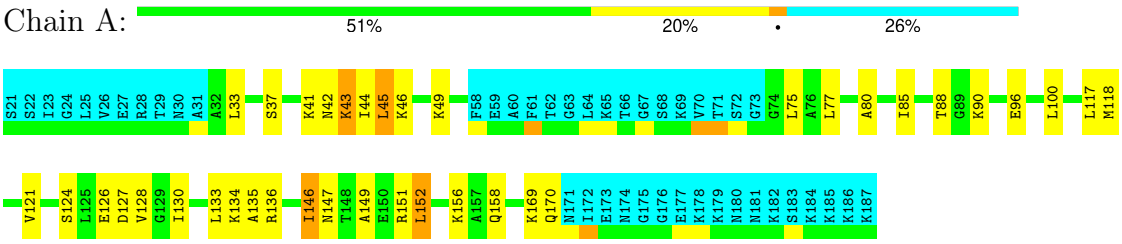
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Decorin-binding protein B

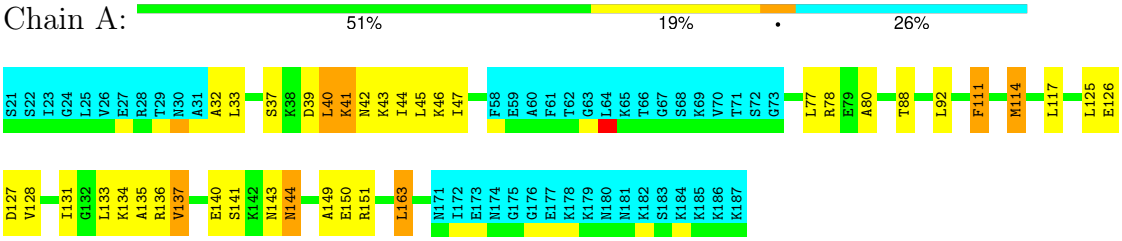
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Decorin-binding protein B

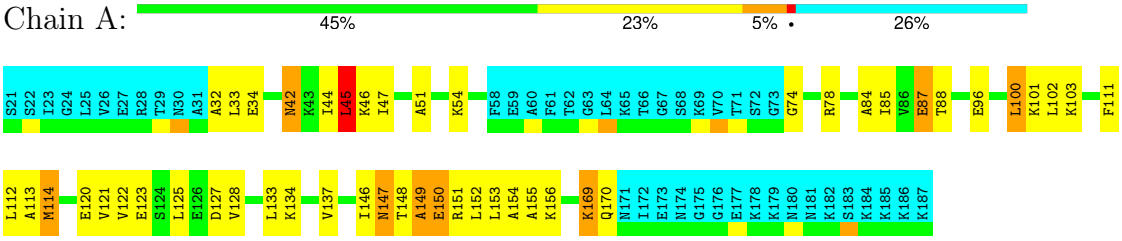
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Decorin-binding protein B

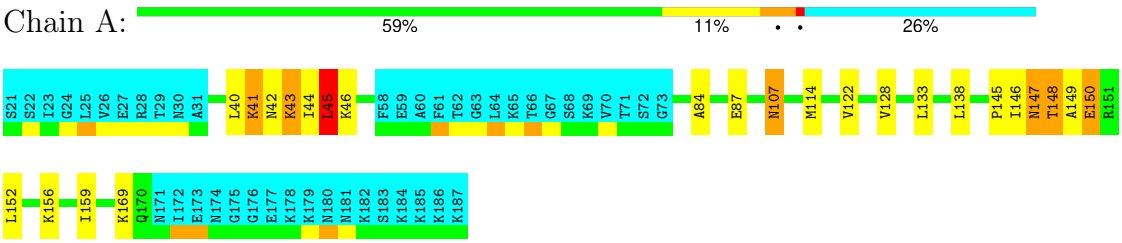
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Decorin-binding protein B

Chain A:



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
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	1888
Number of shifts mapped to atoms	1888
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	947	1029	1029	33±10
All	All	9470	10290	10290	332

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD13	1:A:46:LYS:N	0.83	1.87	9	2
1:A:125:LEU:O	1:A:128:VAL:HG22	0.76	1.79	5	1
1:A:146:ILE:O	1:A:148:THR:N	0.75	2.19	10	1
1:A:42:ASN:O	1:A:45:LEU:HD12	0.73	1.82	3	2
1:A:45:LEU:HD13	1:A:46:LYS:H	0.67	1.48	3	2
1:A:161:ASN:O	1:A:165:VAL:HG23	0.66	1.91	2	2
1:A:143:ASN:ND2	1:A:144:ASN:N	0.63	2.46	3	1
1:A:102:LEU:HD21	1:A:110:GLN:NE2	0.63	2.08	5	1
1:A:121:VAL:HG23	1:A:122:VAL:N	0.61	2.11	9	4
1:A:163:LEU:O	1:A:163:LEU:HD12	0.61	1.95	3	1
1:A:45:LEU:C	1:A:45:LEU:HD22	0.60	2.15	3	2
1:A:40:LEU:HD23	1:A:40:LEU:O	0.60	1.97	2	1
1:A:75:LEU:HD22	1:A:75:LEU:N	0.59	2.12	1	2
1:A:45:LEU:C	1:A:45:LEU:HD12	0.59	2.18	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ASN:O	1:A:45:LEU:HD22	0.58	1.98	10	5
1:A:149:ALA:O	1:A:152:LEU:N	0.58	2.36	1	4
1:A:42:ASN:ND2	1:A:43:LYS:N	0.58	2.52	4	3
1:A:140:GLU:O	1:A:143:ASN:ND2	0.57	2.37	3	2
1:A:147:ASN:HD22	1:A:147:ASN:N	0.57	1.98	9	1
1:A:121:VAL:HG23	1:A:122:VAL:H	0.57	1.59	9	1
1:A:144:ASN:HD21	1:A:151:ARG:NH2	0.56	1.99	1	2
1:A:125:LEU:N	1:A:125:LEU:HD12	0.56	2.16	2	1
1:A:92:LEU:C	1:A:92:LEU:HD12	0.56	2.20	2	1
1:A:117:LEU:C	1:A:117:LEU:HD23	0.55	2.22	1	2
1:A:40:LEU:HD13	1:A:40:LEU:O	0.54	2.02	3	3
1:A:42:ASN:HD22	1:A:43:LYS:N	0.54	1.99	2	2
1:A:44:ILE:O	1:A:46:LYS:N	0.54	2.40	3	8
1:A:134:LYS:O	1:A:137:VAL:N	0.53	2.41	1	8
1:A:147:ASN:HD22	1:A:147:ASN:H	0.53	1.44	9	1
1:A:44:ILE:HD12	1:A:44:ILE:N	0.53	2.18	3	9
1:A:148:THR:OG1	1:A:151:ARG:NE	0.53	2.42	9	1
1:A:40:LEU:O	1:A:43:LYS:N	0.53	2.43	10	3
1:A:132:GLY:O	1:A:133:LEU:CB	0.52	2.57	5	1
1:A:37:SER:CB	1:A:117:LEU:HD11	0.52	2.34	7	2
1:A:163:LEU:C	1:A:163:LEU:HD12	0.52	2.25	8	1
1:A:147:ASN:N	1:A:147:ASN:ND2	0.52	2.58	9	1
1:A:143:ASN:HD22	1:A:144:ASN:N	0.52	2.02	3	1
1:A:41:LYS:H	1:A:41:LYS:CD	0.52	2.17	5	5
1:A:44:ILE:O	1:A:47:ILE:N	0.51	2.43	6	6
1:A:75:LEU:N	1:A:75:LEU:CD2	0.51	2.73	1	2
1:A:37:SER:HB3	1:A:117:LEU:HD11	0.51	1.81	7	1
1:A:152:LEU:HD13	1:A:152:LEU:O	0.51	2.04	9	3
1:A:41:LYS:N	1:A:41:LYS:CD	0.51	2.74	3	1
1:A:156:LYS:O	1:A:159:ILE:N	0.51	2.43	1	4
1:A:148:THR:O	1:A:149:ALA:HB2	0.51	2.04	3	2
1:A:148:THR:O	1:A:149:ALA:CB	0.51	2.58	9	3
1:A:45:LEU:HD23	1:A:46:LYS:N	0.51	2.21	10	5
1:A:148:THR:OG1	1:A:149:ALA:N	0.51	2.42	2	1
1:A:45:LEU:HD22	1:A:45:LEU:O	0.50	2.07	9	1
1:A:84:ALA:O	1:A:87:GLU:N	0.50	2.44	9	5
1:A:134:LYS:O	1:A:136:ARG:N	0.50	2.44	5	5
1:A:118:MET:O	1:A:121:VAL:HG22	0.50	2.06	5	1
1:A:148:THR:O	1:A:150:GLU:N	0.50	2.44	6	1
1:A:107:ASN:HD22	1:A:107:ASN:N	0.50	2.04	3	1
1:A:100:LEU:HD23	1:A:100:LEU:O	0.50	2.06	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HD23	1:A:40:LEU:C	0.49	2.27	2	1
1:A:44:ILE:N	1:A:44:ILE:CD1	0.49	2.74	3	7
1:A:39:ASP:O	1:A:43:LYS:N	0.49	2.44	8	2
1:A:125:LEU:N	1:A:125:LEU:CD1	0.49	2.75	2	1
1:A:131:ILE:O	1:A:132:GLY:C	0.49	2.50	4	1
1:A:125:LEU:O	1:A:127:ASP:N	0.49	2.45	8	5
1:A:41:LYS:CD	1:A:41:LYS:N	0.49	2.76	6	2
1:A:145:PRO:O	1:A:151:ARG:NH1	0.49	2.46	2	1
1:A:143:ASN:HD22	1:A:144:ASN:H	0.49	1.51	3	1
1:A:131:ILE:N	1:A:131:ILE:HD13	0.48	2.23	6	2
1:A:114:MET:C	1:A:114:MET:SD	0.48	2.92	9	2
1:A:140:GLU:OE2	1:A:158:GLN:NE2	0.48	2.46	1	1
1:A:145:PRO:O	1:A:147:ASN:N	0.48	2.47	10	1
1:A:44:ILE:C	1:A:46:LYS:N	0.48	2.67	8	7
1:A:75:LEU:N	1:A:75:LEU:HD12	0.48	2.22	6	3
1:A:144:ASN:HD21	1:A:151:ARG:NE	0.48	2.06	8	1
1:A:40:LEU:C	1:A:40:LEU:HD23	0.48	2.28	1	1
1:A:148:THR:O	1:A:151:ARG:N	0.48	2.46	6	1
1:A:122:VAL:HG22	1:A:122:VAL:O	0.48	2.08	6	3
1:A:128:VAL:HG23	1:A:130:ILE:HD13	0.48	1.85	4	1
1:A:39:ASP:O	1:A:42:ASN:ND2	0.48	2.47	4	2
1:A:146:ILE:O	1:A:147:ASN:C	0.48	2.52	10	1
1:A:152:LEU:O	1:A:155:ALA:N	0.48	2.45	9	3
1:A:149:ALA:O	1:A:150:GLU:C	0.47	2.53	10	3
1:A:115:PHE:O	1:A:119:LEU:HD23	0.47	2.09	5	1
1:A:96:GLU:N	1:A:96:GLU:OE1	0.47	2.47	1	1
1:A:101:LYS:O	1:A:103:LYS:N	0.47	2.47	1	1
1:A:151:ARG:HE	1:A:151:ARG:C	0.47	2.13	3	1
1:A:141:SER:O	1:A:144:ASN:O	0.47	2.32	4	5
1:A:50:GLU:CG	1:A:51:ALA:N	0.47	2.77	2	1
1:A:43:LYS:O	1:A:45:LEU:N	0.47	2.48	7	2
1:A:146:ILE:O	1:A:147:ASN:CG	0.47	2.54	3	1
1:A:114:MET:SD	1:A:114:MET:O	0.47	2.73	6	6
1:A:151:ARG:O	1:A:154:ALA:HB3	0.47	2.10	1	2
1:A:121:VAL:CG2	1:A:122:VAL:N	0.47	2.78	9	5
1:A:157:ALA:O	1:A:161:ASN:ND2	0.46	2.48	4	3
1:A:37:SER:OG	1:A:117:LEU:HD21	0.46	2.10	8	1
1:A:152:LEU:O	1:A:154:ALA:N	0.46	2.49	9	1
1:A:131:ILE:CD1	1:A:131:ILE:H	0.46	2.24	5	1
1:A:149:ALA:O	1:A:152:LEU:CB	0.46	2.64	2	2
1:A:32:ALA:C	1:A:34:GLU:N	0.46	2.69	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:LEU:O	1:A:92:LEU:HD23	0.46	2.10	5	1
1:A:115:PHE:CE1	1:A:141:SER:OG	0.46	2.68	1	1
1:A:41:LYS:NZ	1:A:120:GLU:CG	0.46	2.78	6	1
1:A:77:LEU:O	1:A:80:ALA:N	0.46	2.47	8	2
1:A:102:LEU:HD21	1:A:110:GLN:HE21	0.46	1.70	5	1
1:A:102:LEU:HD22	1:A:102:LEU:N	0.46	2.26	9	1
1:A:101:LYS:C	1:A:103:LYS:N	0.45	2.70	1	3
1:A:154:ALA:O	1:A:157:ALA:N	0.45	2.49	2	1
1:A:163:LEU:N	1:A:163:LEU:HD12	0.45	2.26	2	1
1:A:152:LEU:HD13	1:A:152:LEU:C	0.45	2.31	9	1
1:A:76:ALA:O	1:A:80:ALA:N	0.45	2.50	4	1
1:A:140:GLU:N	1:A:140:GLU:OE1	0.45	2.46	6	1
1:A:152:LEU:CD2	1:A:152:LEU:N	0.45	2.79	6	1
1:A:45:LEU:C	1:A:45:LEU:CD2	0.45	2.85	3	2
1:A:43:LYS:C	1:A:45:LEU:N	0.45	2.69	2	2
1:A:119:LEU:CD2	1:A:119:LEU:N	0.45	2.80	5	1
1:A:115:PHE:CZ	1:A:141:SER:OG	0.45	2.65	1	1
1:A:46:LYS:O	1:A:49:LYS:N	0.45	2.50	7	1
1:A:150:GLU:C	1:A:152:LEU:N	0.45	2.70	9	1
1:A:131:ILE:O	1:A:133:LEU:N	0.44	2.50	4	1
1:A:47:ILE:CG2	1:A:80:ALA:O	0.44	2.66	3	1
1:A:125:LEU:C	1:A:127:ASP:N	0.44	2.71	3	5
1:A:161:ASN:O	1:A:164:LYS:N	0.44	2.50	3	1
1:A:128:VAL:CG2	1:A:130:ILE:HD12	0.44	2.43	7	1
1:A:40:LEU:HD11	1:A:88:THR:HG22	0.44	1.88	8	1
1:A:96:GLU:HB2	1:A:156:LYS:HZ1	0.44	1.72	9	1
1:A:45:LEU:HD23	1:A:46:LYS:H	0.44	1.72	6	1
1:A:131:ILE:O	1:A:132:GLY:O	0.44	2.36	5	1
1:A:39:ASP:O	1:A:42:ASN:OD1	0.44	2.36	3	1
1:A:150:GLU:CG	1:A:151:ARG:N	0.44	2.80	8	1
1:A:32:ALA:O	1:A:34:GLU:N	0.44	2.51	4	2
1:A:111:PHE:O	1:A:113:ALA:N	0.44	2.51	9	1
1:A:124:SER:C	1:A:126:GLU:H	0.44	2.17	2	1
1:A:134:LYS:C	1:A:136:ARG:N	0.44	2.69	5	5
1:A:38:LYS:O	1:A:42:ASN:OD1	0.43	2.36	5	1
1:A:152:LEU:N	1:A:152:LEU:HD22	0.43	2.28	6	1
1:A:102:LEU:N	1:A:102:LEU:CD2	0.43	2.82	9	2
1:A:52:THR:O	1:A:55:GLY:N	0.43	2.52	4	1
1:A:131:ILE:CD1	1:A:131:ILE:N	0.43	2.81	5	1
1:A:162:GLN:O	1:A:165:VAL:N	0.43	2.52	2	1
1:A:146:ILE:C	1:A:148:THR:H	0.43	2.17	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LEU:C	1:A:104:GLU:N	0.43	2.71	2	1
1:A:144:ASN:HD21	1:A:151:ARG:CZ	0.43	2.26	8	1
1:A:92:LEU:HD12	1:A:92:LEU:O	0.43	2.14	2	1
1:A:90:LYS:CG	1:A:91:PHE:N	0.43	2.81	3	1
1:A:108:SER:O	1:A:112:LEU:N	0.43	2.52	3	1
1:A:121:VAL:CG2	1:A:122:VAL:H	0.43	2.25	9	1
1:A:153:LEU:HD12	1:A:153:LEU:N	0.43	2.29	4	1
1:A:152:LEU:C	1:A:154:ALA:N	0.43	2.71	9	2
1:A:161:ASN:N	1:A:161:ASN:HD22	0.43	2.12	4	1
1:A:78:ARG:NH2	1:A:170:GLN:OE1	0.43	2.50	9	1
1:A:138:LEU:HD12	1:A:138:LEU:N	0.43	2.29	1	1
1:A:75:LEU:N	1:A:75:LEU:CD1	0.42	2.81	6	2
1:A:107:ASN:N	1:A:107:ASN:ND2	0.42	2.66	3	1
1:A:169:LYS:N	1:A:169:LYS:CD	0.42	2.82	9	1
1:A:52:THR:O	1:A:53:GLY:C	0.42	2.58	4	1
1:A:51:ALA:O	1:A:54:LYS:N	0.42	2.47	9	1
1:A:111:PHE:C	1:A:113:ALA:N	0.42	2.72	9	1
1:A:120:GLU:O	1:A:123:GLU:CB	0.42	2.67	9	1
1:A:148:THR:OG1	1:A:151:ARG:CZ	0.42	2.67	9	1
1:A:41:LYS:HZ2	1:A:121:VAL:N	0.42	2.13	1	1
1:A:34:GLU:O	1:A:37:SER:OG	0.42	2.36	6	1
1:A:111:PHE:CE2	1:A:149:ALA:HB2	0.42	2.50	8	1
1:A:102:LEU:N	1:A:102:LEU:HD22	0.42	2.29	2	1
1:A:44:ILE:O	1:A:45:LEU:C	0.42	2.58	6	1
1:A:130:ILE:O	1:A:130:ILE:HG23	0.41	2.15	2	1
1:A:125:LEU:N	1:A:125:LEU:HD22	0.41	2.29	9	1
1:A:45:LEU:C	1:A:45:LEU:CD1	0.41	2.87	2	1
1:A:156:LYS:O	1:A:160:GLU:OE1	0.41	2.39	2	1
1:A:152:LEU:O	1:A:152:LEU:HD13	0.41	2.16	1	1
1:A:42:ASN:O	1:A:44:ILE:N	0.41	2.53	4	1
1:A:148:THR:C	1:A:150:GLU:N	0.41	2.71	6	1
1:A:118:MET:O	1:A:121:VAL:CG2	0.41	2.68	7	1
1:A:34:GLU:CD	1:A:35:SER:N	0.41	2.74	5	1
1:A:137:VAL:O	1:A:140:GLU:OE1	0.41	2.39	6	1
1:A:42:ASN:HD22	1:A:42:ASN:C	0.41	2.19	6	1
1:A:117:LEU:HD23	1:A:117:LEU:C	0.41	2.36	6	1
1:A:85:ILE:O	1:A:88:THR:N	0.41	2.54	7	1
1:A:85:ILE:O	1:A:88:THR:OG1	0.41	2.31	9	1
1:A:147:ASN:C	1:A:148:THR:OG1	0.41	2.59	10	1
1:A:85:ILE:HG22	1:A:163:LEU:HD13	0.41	1.91	3	1
1:A:162:GLN:O	1:A:162:GLN:NE2	0.41	2.53	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:GLN:NE2	1:A:162:GLN:C	0.41	2.74	3	1
1:A:127:ASP:N	1:A:127:ASP:OD1	0.41	2.53	7	1
1:A:125:LEU:N	1:A:125:LEU:CD2	0.40	2.83	9	1
1:A:150:GLU:O	1:A:152:LEU:N	0.40	2.54	9	1
1:A:49:LYS:O	1:A:52:THR:N	0.40	2.52	2	1
1:A:92:LEU:C	1:A:92:LEU:CD1	0.40	2.87	2	1
1:A:42:ASN:C	1:A:44:ILE:N	0.40	2.75	4	1
1:A:124:SER:C	1:A:126:GLU:N	0.40	2.74	7	1
1:A:34:GLU:OE2	1:A:35:SER:N	0.40	2.54	3	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	123/167 (74%)	103±4 (84±3%)	15±3 (12±3%)	5±2 (4±1%)	4	29
All	All	1230/1670 (74%)	1031 (84%)	148 (12%)	51 (4%)	4	29

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

Mol	Chain	Res	Type	Models (Total)
1	A	45	LEU	8
1	A	135	ALA	5
1	A	128	VAL	5
1	A	126	GLU	4
1	A	147	ASN	4
1	A	149	ALA	4
1	A	44	ILE	2
1	A	150	GLU	2
1	A	33	LEU	2
1	A	132	GLY	2
1	A	133	LEU	2
1	A	102	LEU	1
1	A	170	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	43	LYS	1
1	A	53	GLY	1
1	A	131	ILE	1
1	A	146	ILE	1
1	A	32	ALA	1
1	A	74	GLY	1
1	A	112	LEU	1
1	A	153	LEU	1
1	A	107	ASN	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	103/139 (74%)	93±2 (90±2%)	10±2 (10±2%)	9 56
All	All	1030/1390 (74%)	931 (90%)	99 (10%)	9 56

All 41 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	133	LEU	8
1	A	45	LEU	7
1	A	43	LYS	6
1	A	41	LYS	5
1	A	131	ILE	5
1	A	42	ASN	5
1	A	148	THR	4
1	A	40	LEU	4
1	A	137	VAL	4
1	A	114	MET	4
1	A	111	PHE	3
1	A	128	VAL	3
1	A	152	LEU	3
1	A	92	LEU	3
1	A	100	LEU	3
1	A	96	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	102	LEU	2
1	A	151	ARG	2
1	A	158	GLN	2
1	A	163	LEU	2
1	A	169	LYS	2
1	A	104	GLU	1
1	A	168	GLU	1
1	A	34	GLU	1
1	A	94	ILE	1
1	A	143	ASN	1
1	A	75	LEU	1
1	A	121	VAL	1
1	A	98	GLU	1
1	A	112	LEU	1
1	A	134	LYS	1
1	A	90	LYS	1
1	A	146	ILE	1
1	A	156	LYS	1
1	A	170	GLN	1
1	A	144	ASN	1
1	A	87	GLU	1
1	A	147	ASN	1
1	A	150	GLU	1
1	A	107	ASN	1
1	A	138	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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% 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: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1888
Number of shifts mapped to atoms	1888
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	166	-1.17 ± 0.26	Should be checked
$^{13}C_{\beta}$	150	0.51 ± 0.10	Should be checked
$^{13}C'$	160	-0.73 ± 0.40	None needed (imprecise)
^{15}N	161	0.18 ± 0.12	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 84%, i.e. 1448 atoms were assigned a chemical shift out of a possible 1724. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	609/621 (98%)	248/253 (98%)	241/246 (98%)	120/122 (98%)
Sidechain	833/1073 (78%)	528/697 (76%)	295/338 (87%)	10/38 (26%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	6/30 (20%)	6/15 (40%)	0/15 (0%)	0/0 (—%)
Overall	1448/1724 (84%)	782/965 (81%)	536/599 (89%)	130/160 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1888 atoms were assigned a chemical shift out of a possible 2293. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	819/847 (97%)	332/347 (96%)	326/334 (98%)	161/166 (97%)
Sidechain	1061/1396 (76%)	664/902 (74%)	385/439 (88%)	12/55 (22%)
Aromatic	8/50 (16%)	8/25 (32%)	0/25 (0%)	0/0 (—%)
Overall	1888/2293 (82%)	1004/1274 (79%)	711/798 (89%)	173/221 (78%)

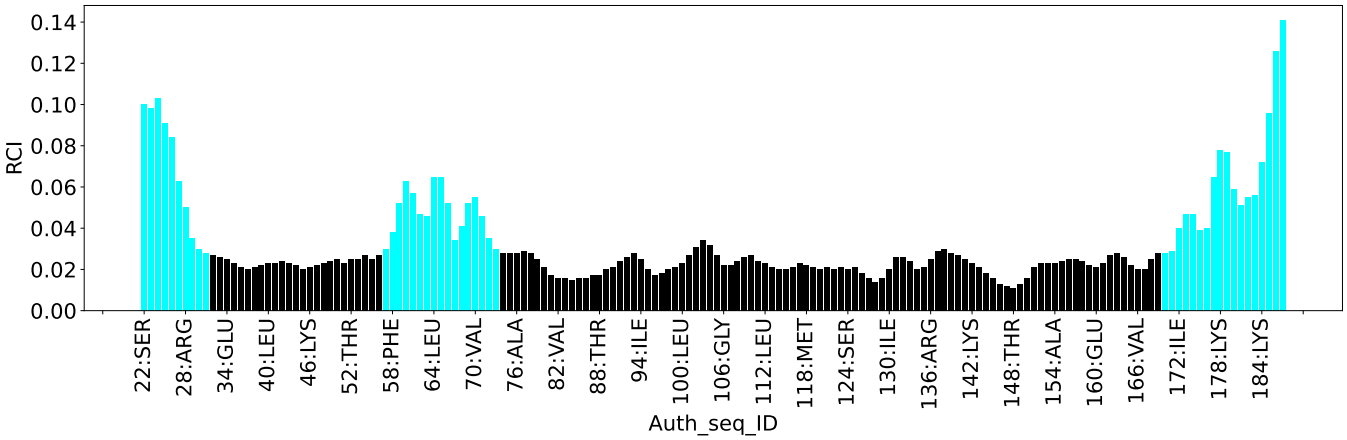
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1699
Intra-residue (|i-j|=0)	538
Sequential (|i-j|=1)	487
Medium range (|i-j|>1 and |i-j|<5)	389
Long range (|i-j|≥5)	285
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	240
Number of unmapped restraints	0
Number of restraints per residue	11.6
Number of long range restraints per residue[1]	1.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	50.9	0.2
0.2-0.5 (Medium)	41.1	0.5
>0.5 (Large)	0.9	0.87

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)	21.5	9.92
10.0-20.0 (Medium)	0.5	14.4
>20.0 (Large)	None	None

9 Distance violation analysis (i)

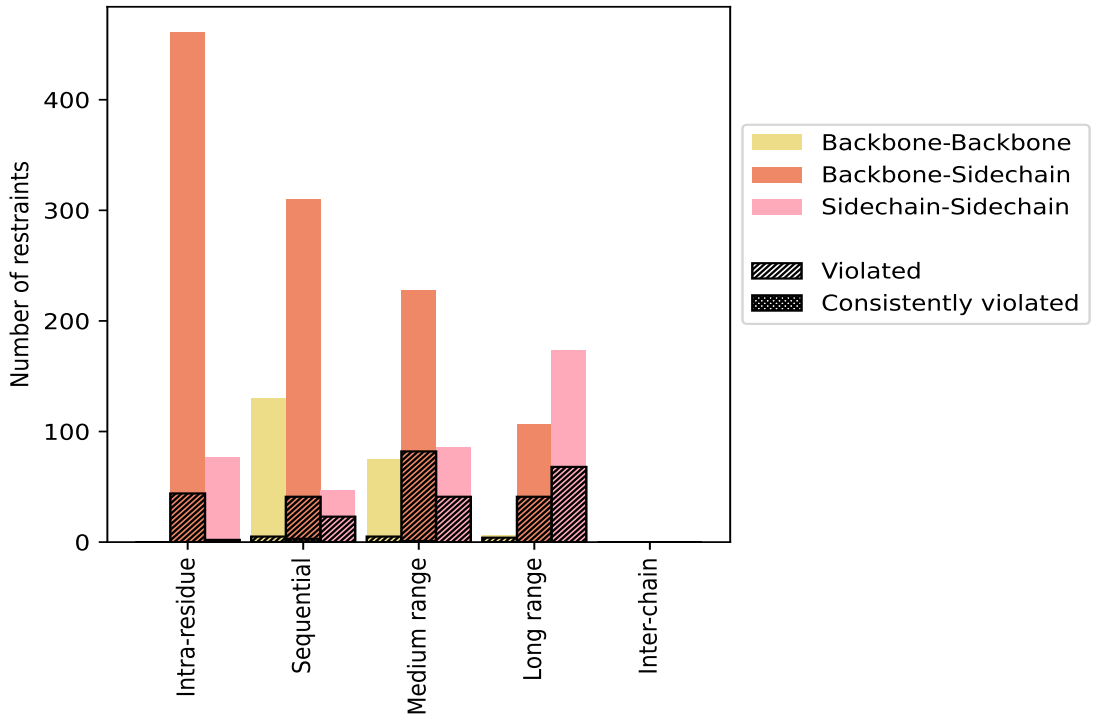
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	538	31.7	46	8.6	2.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	461	27.1	44	9.5	2.6	0	0.0	0.0
Sidechain-Sidechain	77	4.5	2	2.6	0.1	0	0.0	0.0
Sequential (|i-j|=1)	487	28.7	69	14.2	4.1	3	0.6	0.2
Backbone-Backbone	130	7.7	5	3.8	0.3	0	0.0	0.0
Backbone-Sidechain	310	18.2	41	13.2	2.4	3	1.0	0.2
Sidechain-Sidechain	47	2.8	23	48.9	1.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	389	22.9	128	32.9	7.5	1	0.3	0.1
Backbone-Backbone	75	4.4	5	6.7	0.3	0	0.0	0.0
Backbone-Sidechain	228	13.4	82	36.0	4.8	1	0.4	0.1
Sidechain-Sidechain	86	5.1	41	47.7	2.4	0	0.0	0.0
Long range (|i-j|≥5)	285	16.8	113	39.6	6.7	0	0.0	0.0
Backbone-Backbone	6	0.4	4	66.7	0.2	0	0.0	0.0
Backbone-Sidechain	106	6.2	41	38.7	2.4	0	0.0	0.0
Sidechain-Sidechain	173	10.2	68	39.3	4.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1699	100.0	356	21.0	21.0	4	0.2	0.2
Backbone-Backbone	211	12.4	14	6.6	0.8	0	0.0	0.0
Backbone-Sidechain	1105	65.0	208	18.8	12.2	4	0.4	0.2
Sidechain-Sidechain	383	22.5	134	35.0	7.9	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



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

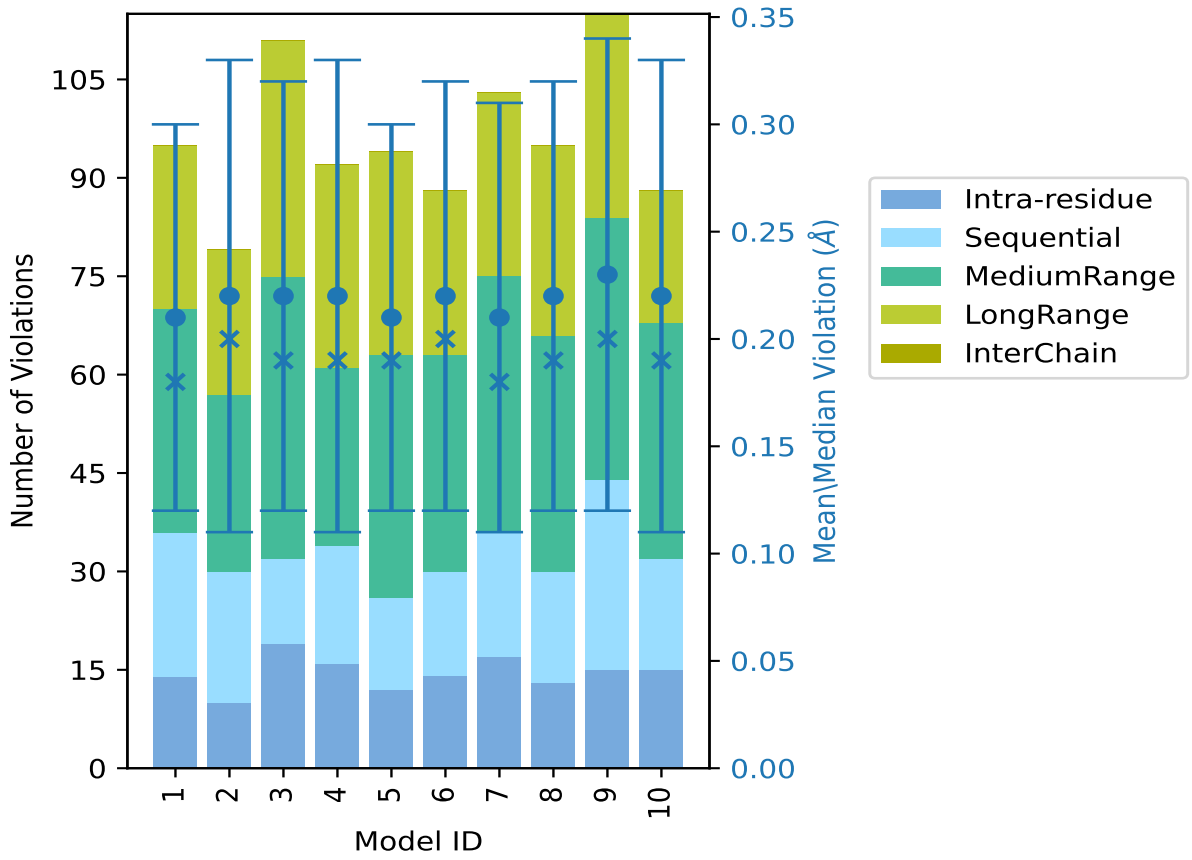
9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	14	22	34	25	0	95	0.21	0.45	0.09	0.18
2	10	20	27	22	0	79	0.22	0.62	0.11	0.2
3	19	13	43	36	0	111	0.22	0.52	0.1	0.19
4	16	18	27	31	0	92	0.22	0.6	0.11	0.19
5	12	14	37	31	0	94	0.21	0.54	0.09	0.19
6	14	16	33	25	0	88	0.22	0.87	0.1	0.2
7	17	19	39	28	0	103	0.21	0.79	0.1	0.18
8	13	17	36	29	0	95	0.22	0.55	0.1	0.19
9	15	29	40	31	0	115	0.23	0.57	0.11	0.2
10	15	17	36	20	0	88	0.22	0.79	0.11	0.19

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

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, 1343(IR:492, SQ:418, MR:261, LR:172, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
16	29	48	51	0	144	1	10.0
11	18	26	26	0	81	2	20.0
6	5	19	12	0	42	3	30.0

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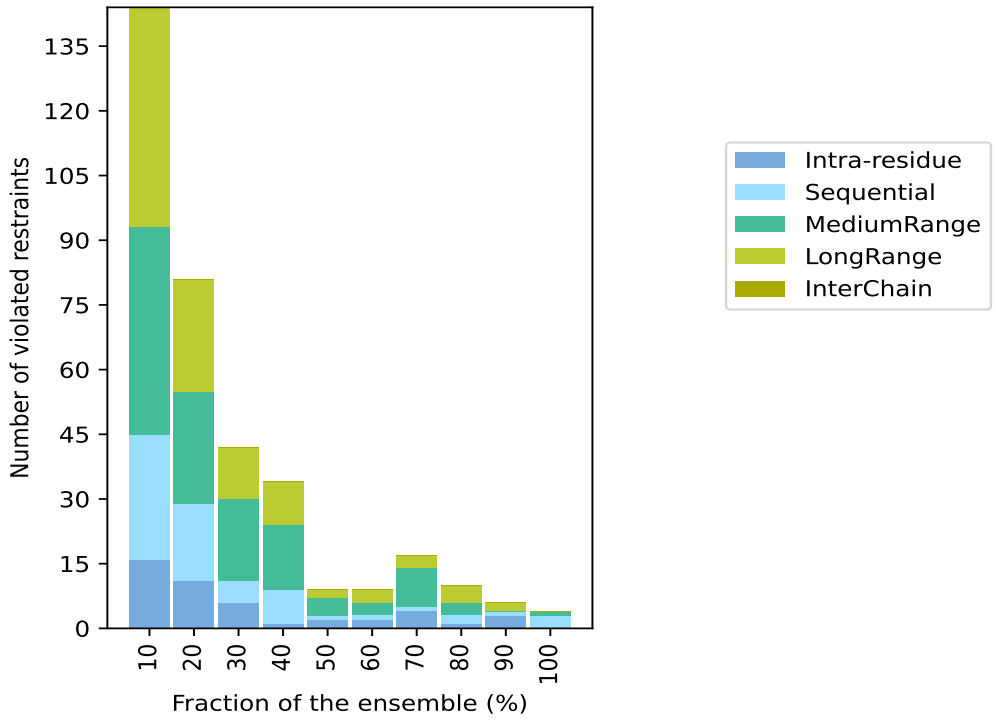
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	8	15	10	0	34	4	40.0
2	1	4	2	0	9	5	50.0
2	1	3	3	0	9	6	60.0
4	1	9	3	0	17	7	70.0
1	2	3	4	0	10	8	80.0
3	1	0	2	0	6	9	90.0
0	3	1	0	0	4	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble

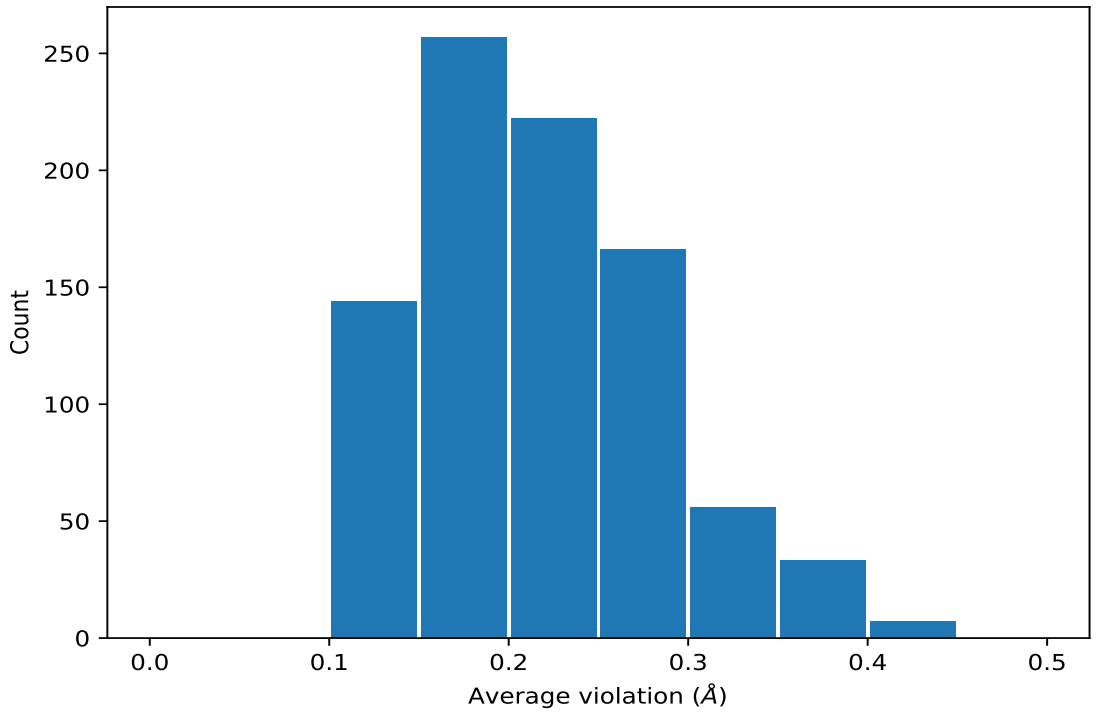


9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

in the ensemble



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	10	0.32	0.09	0.32
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	10	0.32	0.09	0.32
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	10	0.23	0.04	0.23
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	10	0.23	0.04	0.23
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	10	0.23	0.04	0.23
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	10	0.17	0.04	0.18
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	10	0.17	0.04	0.18
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	10	0.15	0.02	0.15
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	9	0.29	0.06	0.3
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	9	0.29	0.06	0.3
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	9	0.29	0.06	0.3
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	9	0.29	0.11	0.26
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	9	0.21	0.06	0.21
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	9	0.21	0.06	0.21
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	9	0.21	0.06	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	9	0.18	0.05	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	9	0.18	0.05	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	9	0.16	0.01	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	9	0.16	0.01	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	9	0.16	0.01	0.16
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	9	0.15	0.01	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	9	0.15	0.01	0.15
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	8	0.31	0.2	0.25
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	8	0.31	0.2	0.25
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	8	0.31	0.2	0.25
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	8	0.31	0.2	0.25
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	8	0.31	0.2	0.25
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	8	0.31	0.2	0.25
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	8	0.26	0.1	0.24
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	8	0.26	0.1	0.24
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	8	0.26	0.1	0.24
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	8	0.26	0.1	0.24
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	8	0.26	0.1	0.24
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	8	0.26	0.1	0.24
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	8	0.24	0.11	0.2
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	8	0.24	0.11	0.2
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	8	0.24	0.11	0.2
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	8	0.23	0.11	0.18
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	8	0.23	0.11	0.18
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	8	0.23	0.11	0.18
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	8	0.23	0.11	0.18
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	8	0.23	0.11	0.18
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	8	0.23	0.11	0.18
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	8	0.23	0.06	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	8	0.23	0.06	0.22
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	8	0.23	0.06	0.22
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	8	0.22	0.07	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	8	0.22	0.07	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	8	0.22	0.07	0.2
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	8	0.22	0.08	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	8	0.2	0.03	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	8	0.2	0.03	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	8	0.2	0.03	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	8	0.2	0.03	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	8	0.2	0.03	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	8	0.2	0.03	0.2
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	8	0.2	0.06	0.2
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	8	0.2	0.06	0.2
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	8	0.2	0.06	0.2
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	8	0.2	0.06	0.2
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	8	0.2	0.06	0.2
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	8	0.2	0.06	0.2
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	8	0.17	0.04	0.18
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	8	0.17	0.04	0.18
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	7	0.39	0.08	0.43
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	7	0.39	0.08	0.43
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	7	0.34	0.1	0.32
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	7	0.34	0.1	0.32
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	7	0.34	0.1	0.32
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	7	0.34	0.1	0.32
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	7	0.34	0.1	0.32
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	7	0.34	0.1	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	7	0.34	0.21	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	7	0.34	0.21	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	7	0.34	0.21	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	7	0.34	0.21	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	7	0.34	0.21	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	7	0.34	0.21	0.32
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	7	0.32	0.09	0.36
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	7	0.32	0.09	0.36
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	7	0.32	0.09	0.36
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	7	0.3	0.07	0.29
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	7	0.29	0.08	0.29
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	7	0.29	0.08	0.29
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	7	0.24	0.07	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	7	0.24	0.07	0.23
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	7	0.23	0.08	0.22
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	7	0.23	0.08	0.22
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	7	0.21	0.09	0.21
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	7	0.21	0.09	0.21
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	7	0.21	0.09	0.21
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	7	0.21	0.1	0.18
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	7	0.21	0.1	0.18
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	7	0.21	0.1	0.18
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	7	0.19	0.07	0.19
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	7	0.18	0.06	0.17
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	7	0.18	0.06	0.17
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	7	0.18	0.06	0.17
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	7	0.18	0.07	0.16
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	7	0.17	0.04	0.17
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	7	0.17	0.04	0.17
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	7	0.16	0.05	0.17
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	7	0.16	0.05	0.17
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	7	0.16	0.05	0.17
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	7	0.16	0.05	0.17
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	7	0.15	0.03	0.16
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	7	0.15	0.03	0.16
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	7	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	7	0.15	0.03	0.15
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	7	0.15	0.03	0.15
(1,739)	1:131:A:ILE:HB	1:132:A:GLY:HA3	6	0.41	0.12	0.38
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB2	6	0.33	0.08	0.34
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB3	6	0.33	0.08	0.34
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG2	6	0.28	0.05	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG3	6	0.28	0.05	0.32
(1,1219)	1:146:A:ILE:HD11	1:149:A:ALA:H	6	0.28	0.09	0.29
(1,1219)	1:146:A:ILE:HD12	1:149:A:ALA:H	6	0.28	0.09	0.29
(1,1219)	1:146:A:ILE:HD13	1:149:A:ALA:H	6	0.28	0.09	0.29
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG2	6	0.24	0.05	0.23
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG3	6	0.24	0.05	0.23
(1,1195)	1:111:A:PHE:H	1:147:A:ASN:HA	6	0.21	0.07	0.22
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD11	6	0.21	0.07	0.19
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD12	6	0.21	0.07	0.19
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD13	6	0.21	0.07	0.19
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD21	6	0.19	0.04	0.18
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD22	6	0.19	0.04	0.18
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD23	6	0.19	0.04	0.18
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD11	6	0.16	0.09	0.13
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD12	6	0.16	0.09	0.13
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD13	6	0.16	0.09	0.13
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD21	5	0.31	0.02	0.3
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD22	5	0.31	0.02	0.3
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD23	5	0.31	0.02	0.3
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB2	5	0.28	0.16	0.22
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB3	5	0.28	0.16	0.22
(1,18)	1:25:A:LEU:HB2	1:26:A:VAL:HA	5	0.26	0.11	0.25
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD11	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD12	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD13	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD21	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD22	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD23	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD11	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD12	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD13	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD21	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD22	5	0.26	0.04	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD23	5	0.26	0.04	0.24
(1,694)	1:114:A:MET:HE1	1:118:A:MET:HB3	5	0.24	0.13	0.18
(1,694)	1:114:A:MET:HE2	1:118:A:MET:HB3	5	0.24	0.13	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,694)	1:114:A:MET:HE3	1:118:A:MET:HB3	5	0.24	0.13	0.18
(1,318)	1:102:A:LEU:HD11	1:106:A:GLY:H	5	0.22	0.09	0.2
(1,318)	1:102:A:LEU:HD12	1:106:A:GLY:H	5	0.22	0.09	0.2
(1,318)	1:102:A:LEU:HD13	1:106:A:GLY:H	5	0.22	0.09	0.2
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD11	5	0.18	0.05	0.21
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD12	5	0.18	0.05	0.21
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD13	5	0.18	0.05	0.21
(1,755)	1:44:A:ILE:HD11	1:124:A:SER:H	5	0.17	0.05	0.14
(1,755)	1:44:A:ILE:HD12	1:124:A:SER:H	5	0.17	0.05	0.14
(1,755)	1:44:A:ILE:HD13	1:124:A:SER:H	5	0.17	0.05	0.14
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD2	5	0.16	0.05	0.16
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD3	5	0.16	0.05	0.16
(1,1151)	1:141:A:SER:H	1:146:A:ILE:HB	4	0.37	0.09	0.36
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB2	4	0.34	0.13	0.29
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB3	4	0.34	0.13	0.29
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB2	4	0.34	0.13	0.29
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB3	4	0.34	0.13	0.29
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD11	4	0.33	0.18	0.34
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD12	4	0.33	0.18	0.34
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD13	4	0.33	0.18	0.34
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD11	4	0.33	0.18	0.34
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD12	4	0.33	0.18	0.34
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD13	4	0.33	0.18	0.34
(1,618)	1:146:A:ILE:HG21	1:152:A:LEU:HA	4	0.32	0.12	0.28
(1,618)	1:146:A:ILE:HG22	1:152:A:LEU:HA	4	0.32	0.12	0.28
(1,618)	1:146:A:ILE:HG23	1:152:A:LEU:HA	4	0.32	0.12	0.28
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG21	4	0.29	0.1	0.28
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG22	4	0.29	0.1	0.28
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG23	4	0.29	0.1	0.28
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG21	4	0.29	0.1	0.28
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG22	4	0.29	0.1	0.28
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG23	4	0.29	0.1	0.28
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD11	4	0.29	0.06	0.29
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD12	4	0.29	0.06	0.29
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD13	4	0.29	0.06	0.29
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD21	4	0.29	0.06	0.29
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD22	4	0.29	0.06	0.29
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD23	4	0.29	0.06	0.29
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG11	4	0.28	0.1	0.28
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG12	4	0.28	0.1	0.28
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG13	4	0.28	0.1	0.28
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG21	4	0.28	0.1	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG22	4	0.28	0.1	0.28
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG23	4	0.28	0.1	0.28
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG21	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG22	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG23	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG21	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG22	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG23	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG21	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG22	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG23	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG21	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG22	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG23	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG21	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG22	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG23	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG21	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG22	4	0.28	0.11	0.27
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG23	4	0.28	0.11	0.27
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA2	4	0.27	0.07	0.28
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA3	4	0.27	0.07	0.28
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA2	4	0.27	0.07	0.28
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA3	4	0.27	0.07	0.28
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA2	4	0.27	0.07	0.28
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA3	4	0.27	0.07	0.28
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB2	4	0.27	0.06	0.28
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB3	4	0.27	0.06	0.28
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG21	4	0.24	0.09	0.23
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG22	4	0.24	0.09	0.23
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG23	4	0.24	0.09	0.23
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB2	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB3	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB2	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB3	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB2	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB3	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB2	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB3	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB2	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB3	4	0.22	0.13	0.17
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB2	4	0.22	0.13	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB3	4	0.22	0.13	0.17
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG2	4	0.22	0.06	0.22
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG3	4	0.22	0.06	0.22
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG2	4	0.22	0.06	0.22
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG3	4	0.22	0.06	0.22
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG2	4	0.22	0.08	0.22
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG3	4	0.22	0.08	0.22
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG2	4	0.22	0.08	0.22
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG3	4	0.22	0.08	0.22
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG2	4	0.22	0.08	0.22
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG3	4	0.22	0.08	0.22
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB2	4	0.22	0.04	0.22
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB3	4	0.22	0.04	0.22
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG11	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG12	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG13	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG21	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG22	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG23	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG11	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG12	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG13	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG21	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG22	4	0.22	0.14	0.15
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG23	4	0.22	0.14	0.15
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB2	4	0.21	0.08	0.2
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB3	4	0.21	0.08	0.2
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB2	4	0.21	0.08	0.2
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB3	4	0.21	0.08	0.2
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG2	4	0.21	0.09	0.21
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG3	4	0.21	0.09	0.21
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD2	4	0.21	0.03	0.2
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD3	4	0.21	0.03	0.2
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	4	0.2	0.07	0.18
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	4	0.2	0.07	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,478)	1:99:A:ALA:HB1	1:153:A:LEU:HG	4	0.19	0.08	0.18
(1,478)	1:99:A:ALA:HB2	1:153:A:LEU:HG	4	0.19	0.08	0.18
(1,478)	1:99:A:ALA:HB3	1:153:A:LEU:HG	4	0.19	0.08	0.18
(1,204)	1:77:A:LEU:HG	1:81:A:LYS:H	4	0.18	0.04	0.18
(1,748)	1:39:A:ASP:HA	1:42:A:ASN:HD22	4	0.18	0.06	0.17
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD11	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD12	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD13	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD21	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD22	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD23	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD11	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD12	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD13	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD21	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD22	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD23	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD11	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD12	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD13	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD21	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD22	4	0.18	0.04	0.16
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD23	4	0.18	0.04	0.16
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG2	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG3	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG2	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG3	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG2	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG3	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG2	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG3	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG2	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG3	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG2	4	0.18	0.06	0.16
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG3	4	0.18	0.06	0.16
(1,502)	1:63:A:GLY:H	1:66:A:THR:HA	4	0.18	0.03	0.16
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG2	4	0.17	0.05	0.17
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG3	4	0.17	0.05	0.17
(1,1042)	1:121:A:VAL:HB	1:124:A:SER:H	4	0.17	0.09	0.12
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	4	0.17	0.03	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	4	0.17	0.03	0.16
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	4	0.17	0.03	0.16
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG2	4	0.17	0.06	0.16
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG3	4	0.17	0.06	0.16
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG2	4	0.17	0.06	0.16
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG3	4	0.17	0.06	0.16
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE2	4	0.16	0.02	0.17
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE3	4	0.16	0.02	0.17
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE2	4	0.16	0.02	0.17
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE3	4	0.16	0.02	0.17
(1,886)	1:146:A:ILE:HG21	1:149:A:ALA:H	4	0.16	0.02	0.16
(1,886)	1:146:A:ILE:HG22	1:149:A:ALA:H	4	0.16	0.02	0.16
(1,886)	1:146:A:ILE:HG23	1:149:A:ALA:H	4	0.16	0.02	0.16
(1,1147)	1:139:A:GLU:HG2	1:141:A:SER:H	4	0.16	0.02	0.16
(1,1147)	1:139:A:GLU:HG3	1:141:A:SER:H	4	0.16	0.02	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG21	4	0.16	0.01	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG22	4	0.16	0.01	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG23	4	0.16	0.01	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG21	4	0.16	0.01	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG22	4	0.16	0.01	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG23	4	0.16	0.01	0.16
(1,742)	1:131:A:ILE:HD11	1:132:A:GLY:H	3	0.29	0.09	0.32
(1,742)	1:131:A:ILE:HD12	1:132:A:GLY:H	3	0.29	0.09	0.32
(1,742)	1:131:A:ILE:HD13	1:132:A:GLY:H	3	0.29	0.09	0.32
(1,1168)	1:102:A:LEU:HD21	1:106:A:GLY:H	3	0.29	0.07	0.24
(1,1168)	1:102:A:LEU:HD22	1:106:A:GLY:H	3	0.29	0.07	0.24
(1,1168)	1:102:A:LEU:HD23	1:106:A:GLY:H	3	0.29	0.07	0.24
(1,101)	1:83:A:GLN:H	1:83:A:GLN:HG3	3	0.27	0.16	0.17
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG2	3	0.26	0.12	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG3	3	0.26	0.12	0.29
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG2	3	0.26	0.12	0.29
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG3	3	0.26	0.12	0.29
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG2	3	0.26	0.12	0.29
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG3	3	0.26	0.12	0.29
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB2	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB3	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB2	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB3	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB2	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB3	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB2	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB3	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB2	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB3	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB2	3	0.26	0.12	0.2
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB3	3	0.26	0.12	0.2
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE2	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE3	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE2	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE3	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE2	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE3	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE2	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE3	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE2	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE3	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE2	3	0.25	0.11	0.18
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE3	3	0.25	0.11	0.18
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG2	3	0.25	0.09	0.29
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG3	3	0.25	0.09	0.29
(1,1116)	1:101:A:LYS:HD2	1:104:A:GLU:H	3	0.24	0.15	0.14
(1,1116)	1:101:A:LYS:HD3	1:104:A:GLU:H	3	0.24	0.15	0.14
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD11	3	0.24	0.18	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD12	3	0.24	0.18	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD13	3	0.24	0.18	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD21	3	0.24	0.18	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD22	3	0.24	0.18	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD23	3	0.24	0.18	0.12
(1,1517)	1:112:A:LEU:HD11	1:147:A:ASN:HA	3	0.23	0.07	0.2
(1,1517)	1:112:A:LEU:HD12	1:147:A:ASN:HA	3	0.23	0.07	0.2
(1,1517)	1:112:A:LEU:HD13	1:147:A:ASN:HA	3	0.23	0.07	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1517)	1:112:A:LEU:HD21	1:147:A:ASN:HA	3	0.23	0.07	0.2
(1,1517)	1:112:A:LEU:HD22	1:147:A:ASN:HA	3	0.23	0.07	0.2
(1,1517)	1:112:A:LEU:HD23	1:147:A:ASN:HA	3	0.23	0.07	0.2
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE2	3	0.23	0.11	0.22
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE3	3	0.23	0.11	0.22
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE2	3	0.23	0.11	0.22
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE3	3	0.23	0.11	0.22
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG2	3	0.23	0.05	0.22
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG3	3	0.23	0.05	0.22
(1,652)	1:25:A:LEU:HA	1:25:A:LEU:HG	3	0.23	0.04	0.25
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD11	3	0.23	0.05	0.23
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD12	3	0.23	0.05	0.23
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD13	3	0.23	0.05	0.23
(1,1041)	1:159:A:ILE:HB	1:162:A:GLN:H	3	0.23	0.06	0.23
(1,954)	1:26:A:VAL:H	1:26:A:VAL:HB	3	0.22	0.04	0.22
(1,188)	1:153:A:LEU:H	1:153:A:LEU:HG	3	0.22	0.01	0.21
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB1	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB2	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB3	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB1	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB2	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB3	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB1	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB2	3	0.22	0.11	0.18
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB3	3	0.22	0.11	0.18
(1,781)	1:85:A:ILE:HG21	1:88:A:THR:HA	3	0.21	0.03	0.2
(1,781)	1:85:A:ILE:HG22	1:88:A:THR:HA	3	0.21	0.03	0.2
(1,781)	1:85:A:ILE:HG23	1:88:A:THR:HA	3	0.21	0.03	0.2
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG2	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG3	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG2	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG3	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG2	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG3	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG2	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG3	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG2	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG3	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG2	3	0.21	0.11	0.14
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG3	3	0.21	0.11	0.14
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD11	3	0.2	0.02	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD12	3	0.2	0.02	0.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD13	3	0.2	0.02	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD21	3	0.2	0.02	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD22	3	0.2	0.02	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD23	3	0.2	0.02	0.21
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD11	3	0.19	0.06	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD12	3	0.19	0.06	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD13	3	0.19	0.06	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD21	3	0.19	0.06	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD22	3	0.19	0.06	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD23	3	0.19	0.06	0.17
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD11	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD12	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD13	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD21	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD22	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD23	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD11	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD12	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD13	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD21	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD22	3	0.19	0.09	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD23	3	0.19	0.09	0.13
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD2	3	0.18	0.02	0.19
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD3	3	0.18	0.02	0.19
(1,661)	1:157:A:ALA:HA	1:159:A:ILE:H	3	0.17	0.07	0.15
(1,1209)	1:64:A:LEU:HD21	1:67:A:GLY:H	3	0.17	0.07	0.14
(1,1209)	1:64:A:LEU:HD22	1:67:A:GLY:H	3	0.17	0.07	0.14
(1,1209)	1:64:A:LEU:HD23	1:67:A:GLY:H	3	0.17	0.07	0.14
(1,1665)	1:158:A:GLN:HG2	1:161:A:ASN:H	3	0.17	0.04	0.19
(1,1665)	1:158:A:GLN:HG3	1:161:A:ASN:H	3	0.17	0.04	0.19
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE1	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE2	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE3	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE1	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE2	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE3	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE1	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE2	3	0.17	0.02	0.16
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE3	3	0.17	0.02	0.16
(1,56)	1:172:A:ILE:HB	1:173:A:GLU:H	3	0.16	0.04	0.19
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD2	3	0.16	0.0	0.16
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD3	3	0.16	0.0	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG21	3	0.16	0.05	0.13
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG22	3	0.16	0.05	0.13
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG23	3	0.16	0.05	0.13
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG21	3	0.16	0.05	0.13
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG22	3	0.16	0.05	0.13
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG23	3	0.16	0.05	0.13
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG2	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG3	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG2	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG3	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG2	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG3	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG2	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG3	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG2	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG3	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG2	3	0.16	0.04	0.16
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG3	3	0.16	0.04	0.16
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD11	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD12	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD13	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD21	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD22	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD23	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD11	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD12	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD13	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD21	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD22	3	0.16	0.04	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD23	3	0.16	0.04	0.15
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD11	3	0.16	0.05	0.15
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD12	3	0.16	0.05	0.15
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD13	3	0.16	0.05	0.15
(1,1192)	1:146:A:ILE:H	1:148:A:THR:H	3	0.16	0.02	0.17
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD11	3	0.15	0.03	0.14
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD12	3	0.15	0.03	0.14
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD13	3	0.15	0.03	0.14
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD11	3	0.15	0.03	0.14
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD12	3	0.15	0.03	0.14
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD13	3	0.15	0.03	0.14
(1,270)	1:133:A:LEU:HD11	1:165:A:VAL:HB	3	0.15	0.04	0.17
(1,270)	1:133:A:LEU:HD12	1:165:A:VAL:HB	3	0.15	0.04	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,270)	1:133:A:LEU:HD13	1:165:A:VAL:HB	3	0.15	0.04	0.17
(1,642)	1:38:A:LYS:HB2	1:39:A:ASP:HA	3	0.15	0.02	0.16
(1,642)	1:38:A:LYS:HB3	1:39:A:ASP:HA	3	0.15	0.02	0.16
(1,218)	1:109:A:GLY:HA2	1:112:A:LEU:HG	3	0.15	0.03	0.14
(1,218)	1:109:A:GLY:HA3	1:112:A:LEU:HG	3	0.15	0.03	0.14
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD1	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD2	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD1	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD2	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD1	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD2	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD1	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD2	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD1	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD2	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD1	3	0.15	0.06	0.11
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD2	3	0.15	0.06	0.11
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB1	3	0.14	0.04	0.12
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB2	3	0.14	0.04	0.12
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB3	3	0.14	0.04	0.12
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD11	3	0.14	0.05	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD12	3	0.14	0.05	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD13	3	0.14	0.05	0.1
(1,643)	1:54:A:LYS:HA	1:54:A:LYS:HD2	2	0.42	0.01	0.42
(1,643)	1:54:A:LYS:HA	1:54:A:LYS:HD3	2	0.42	0.01	0.42
(1,102)	1:158:A:GLN:H	1:158:A:GLN:HG2	2	0.4	0.17	0.4
(1,191)	1:152:A:LEU:HD21	1:154:A:ALA:H	2	0.4	0.05	0.4
(1,191)	1:152:A:LEU:HD22	1:154:A:ALA:H	2	0.4	0.05	0.4
(1,191)	1:152:A:LEU:HD23	1:154:A:ALA:H	2	0.4	0.05	0.4
(1,1571)	1:128:A:VAL:HG21	1:129:A:GLY:HA2	2	0.39	0.03	0.39
(1,1571)	1:128:A:VAL:HG21	1:129:A:GLY:HA3	2	0.39	0.03	0.39
(1,1571)	1:128:A:VAL:HG22	1:129:A:GLY:HA2	2	0.39	0.03	0.39
(1,1571)	1:128:A:VAL:HG22	1:129:A:GLY:HA3	2	0.39	0.03	0.39
(1,1571)	1:128:A:VAL:HG23	1:129:A:GLY:HA2	2	0.39	0.03	0.39
(1,1571)	1:128:A:VAL:HG23	1:129:A:GLY:HA3	2	0.39	0.03	0.39
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG11	2	0.38	0.02	0.38
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG12	2	0.38	0.02	0.38
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG13	2	0.38	0.02	0.38
(1,542)	1:38:A:LYS:HA	1:38:A:LYS:HE2	2	0.38	0.01	0.38
(1,542)	1:38:A:LYS:HA	1:38:A:LYS:HE3	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD11	1:67:A:GLY:HA2	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD11	1:67:A:GLY:HA3	2	0.38	0.01	0.38

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1385)	1:64:A:LEU:HD12	1:67:A:GLY:HA2	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD12	1:67:A:GLY:HA3	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD13	1:67:A:GLY:HA2	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD13	1:67:A:GLY:HA3	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD21	1:67:A:GLY:HA2	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD21	1:67:A:GLY:HA3	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD22	1:67:A:GLY:HA2	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD22	1:67:A:GLY:HA3	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD23	1:67:A:GLY:HA2	2	0.38	0.01	0.38
(1,1385)	1:64:A:LEU:HD23	1:67:A:GLY:HA3	2	0.38	0.01	0.38
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB1	2	0.37	0.08	0.37
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB2	2	0.37	0.08	0.37
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB3	2	0.37	0.08	0.37
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB1	2	0.37	0.08	0.37
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB2	2	0.37	0.08	0.37
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB3	2	0.37	0.08	0.37
(1,1012)	1:148:A:THR:H	1:151:A:ARG:H	2	0.36	0.06	0.36
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	2	0.34	0.07	0.34
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	2	0.34	0.07	0.34
(1,1309)	1:40:A:LEU:HD11	1:121:A:VAL:HB	2	0.34	0.16	0.34
(1,1309)	1:40:A:LEU:HD12	1:121:A:VAL:HB	2	0.34	0.16	0.34
(1,1309)	1:40:A:LEU:HD13	1:121:A:VAL:HB	2	0.34	0.16	0.34
(1,1309)	1:40:A:LEU:HD21	1:121:A:VAL:HB	2	0.34	0.16	0.34
(1,1309)	1:40:A:LEU:HD22	1:121:A:VAL:HB	2	0.34	0.16	0.34
(1,1309)	1:40:A:LEU:HD23	1:121:A:VAL:HB	2	0.34	0.16	0.34
(1,1233)	1:89:A:GLY:H	1:90:A:LYS:HD2	2	0.3	0.01	0.3
(1,1233)	1:89:A:GLY:H	1:90:A:LYS:HD3	2	0.3	0.01	0.3
(1,1564)	1:122:A:VAL:HG11	1:134:A:LYS:HE2	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG11	1:134:A:LYS:HE3	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG12	1:134:A:LYS:HE2	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG12	1:134:A:LYS:HE3	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG13	1:134:A:LYS:HE2	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG13	1:134:A:LYS:HE3	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG21	1:134:A:LYS:HE2	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG21	1:134:A:LYS:HE3	2	0.3	0.16	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1564)	1:122:A:VAL:HG22	1:134:A:LYS:HE2	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG22	1:134:A:LYS:HE3	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG23	1:134:A:LYS:HE2	2	0.3	0.16	0.3
(1,1564)	1:122:A:VAL:HG23	1:134:A:LYS:HE3	2	0.3	0.16	0.3
(1,1048)	1:37:A:SER:H	1:41:A:LYS:HD2	2	0.3	0.13	0.3
(1,1048)	1:37:A:SER:H	1:41:A:LYS:HD3	2	0.3	0.13	0.3
(1,669)	1:113:A:ALA:HA	1:116:A:ASP:HB3	2	0.3	0.01	0.3
(1,134)	1:44:A:ILE:HA	1:48:A:LYS:HB2	2	0.28	0.14	0.28
(1,134)	1:44:A:ILE:HA	1:48:A:LYS:HB3	2	0.28	0.14	0.28
(1,237)	1:133:A:LEU:HD21	1:162:A:GLN:H	2	0.28	0.1	0.28
(1,237)	1:133:A:LEU:HD22	1:162:A:GLN:H	2	0.28	0.1	0.28
(1,237)	1:133:A:LEU:HD23	1:162:A:GLN:H	2	0.28	0.1	0.28
(1,1376)	1:60:A:ALA:HA	1:64:A:LEU:HB2	2	0.28	0.16	0.28
(1,1376)	1:60:A:ALA:HA	1:64:A:LEU:HB3	2	0.28	0.16	0.28
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD11	2	0.28	0.04	0.28
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD12	2	0.28	0.04	0.28
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD13	2	0.28	0.04	0.28
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD21	2	0.28	0.04	0.28
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD22	2	0.28	0.04	0.28
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD23	2	0.28	0.04	0.28
(1,1232)	1:89:A:GLY:H	1:90:A:LYS:HG2	2	0.26	0.01	0.26
(1,1232)	1:89:A:GLY:H	1:90:A:LYS:HG3	2	0.26	0.01	0.26
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD11	2	0.26	0.1	0.26
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD12	2	0.26	0.1	0.26
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD13	2	0.26	0.1	0.26
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG11	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG12	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG13	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG21	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG22	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG23	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG11	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG12	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG13	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG21	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG22	2	0.26	0.03	0.26
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG23	2	0.26	0.03	0.26
(1,1208)	1:64:A:LEU:HD11	1:67:A:GLY:H	2	0.26	0.08	0.26
(1,1208)	1:64:A:LEU:HD12	1:67:A:GLY:H	2	0.26	0.08	0.26
(1,1208)	1:64:A:LEU:HD13	1:67:A:GLY:H	2	0.26	0.08	0.26
(1,42)	1:37:A:SER:HA	1:39:A:ASP:HB3	2	0.24	0.11	0.24
(1,662)	1:146:A:ILE:HD11	1:155:A:ALA:H	2	0.24	0.12	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,662)	1:146:A:ILE:HD12	1:155:A:ALA:H	2	0.24	0.12	0.24
(1,662)	1:146:A:ILE:HD13	1:155:A:ALA:H	2	0.24	0.12	0.24
(1,52)	1:160:A:GLU:H	1:160:A:GLU:HG3	2	0.23	0.06	0.23
(1,1214)	1:60:A:ALA:H	1:61:A:PHE:HD1	2	0.22	0.01	0.22
(1,1214)	1:60:A:ALA:H	1:61:A:PHE:HD2	2	0.22	0.01	0.22
(1,1184)	1:168:A:GLU:H	1:169:A:LYS:HD2	2	0.22	0.04	0.22
(1,1184)	1:168:A:GLU:H	1:169:A:LYS:HD3	2	0.22	0.04	0.22
(1,1592)	1:133:A:LEU:HD11	1:165:A:VAL:HB	2	0.22	0.02	0.22
(1,1592)	1:133:A:LEU:HD12	1:165:A:VAL:HB	2	0.22	0.02	0.22
(1,1592)	1:133:A:LEU:HD13	1:165:A:VAL:HB	2	0.22	0.02	0.22
(1,1592)	1:133:A:LEU:HD21	1:165:A:VAL:HB	2	0.22	0.02	0.22
(1,1592)	1:133:A:LEU:HD22	1:165:A:VAL:HB	2	0.22	0.02	0.22
(1,1592)	1:133:A:LEU:HD23	1:165:A:VAL:HB	2	0.22	0.02	0.22
(1,499)	1:114:A:MET:HE1	1:156:A:LYS:H	2	0.21	0.05	0.21
(1,499)	1:114:A:MET:HE2	1:156:A:LYS:H	2	0.21	0.05	0.21
(1,499)	1:114:A:MET:HE3	1:156:A:LYS:H	2	0.21	0.05	0.21
(1,41)	1:37:A:SER:HA	1:39:A:ASP:HB2	2	0.2	0.0	0.2
(1,283)	1:29:A:THR:HB	1:30:A:ASN:H	2	0.2	0.0	0.2
(1,1612)	1:137:A:VAL:HB	1:158:A:GLN:HE21	2	0.2	0.02	0.2
(1,1612)	1:137:A:VAL:HB	1:158:A:GLN:HE22	2	0.2	0.02	0.2
(1,1511)	1:112:A:LEU:HB2	1:116:A:ASP:H	2	0.2	0.09	0.2
(1,1511)	1:112:A:LEU:HB3	1:116:A:ASP:H	2	0.2	0.09	0.2
(1,1666)	1:159:A:ILE:HA	1:162:A:GLN:HG2	2	0.2	0.02	0.2
(1,1666)	1:159:A:ILE:HA	1:162:A:GLN:HG3	2	0.2	0.02	0.2
(1,93)	1:139:A:GLU:H	1:139:A:GLU:HG2	2	0.2	0.04	0.2
(1,93)	1:139:A:GLU:H	1:139:A:GLU:HG3	2	0.2	0.04	0.2
(1,174)	1:65:A:LYS:HA	1:65:A:LYS:HD2	2	0.2	0.04	0.2
(1,174)	1:65:A:LYS:HA	1:65:A:LYS:HD3	2	0.2	0.04	0.2
(1,423)	1:131:A:ILE:HG21	1:132:A:GLY:H	2	0.2	0.02	0.2
(1,423)	1:131:A:ILE:HG22	1:132:A:GLY:H	2	0.2	0.02	0.2
(1,423)	1:131:A:ILE:HG23	1:132:A:GLY:H	2	0.2	0.02	0.2
(1,1040)	1:162:A:GLN:H	1:165:A:VAL:HB	2	0.2	0.01	0.2
(1,798)	1:61:A:PHE:HA	1:61:A:PHE:HD1	2	0.19	0.0	0.19
(1,798)	1:61:A:PHE:HA	1:61:A:PHE:HD2	2	0.19	0.0	0.19
(1,176)	1:45:A:LEU:HA	1:48:A:LYS:HD2	2	0.18	0.02	0.18
(1,176)	1:45:A:LEU:HA	1:48:A:LYS:HD3	2	0.18	0.02	0.18
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD11	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD12	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD13	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD21	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD22	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD23	2	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD11	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD12	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD13	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD21	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD22	2	0.18	0.05	0.18
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD23	2	0.18	0.05	0.18
(1,1117)	1:101:A:LYS:HG2	1:104:A:GLU:H	2	0.18	0.06	0.18
(1,1117)	1:101:A:LYS:HG3	1:104:A:GLU:H	2	0.18	0.06	0.18
(1,1140)	1:35:A:SER:H	1:38:A:LYS:HG2	2	0.18	0.04	0.18
(1,1140)	1:35:A:SER:H	1:38:A:LYS:HG3	2	0.18	0.04	0.18
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG11	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG12	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG13	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG21	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG22	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG23	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG11	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG12	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG13	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG21	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG22	2	0.18	0.05	0.18
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG23	2	0.18	0.05	0.18
(1,75)	1:59:A:GLU:HA	1:59:A:GLU:HG2	2	0.18	0.02	0.18
(1,75)	1:59:A:GLU:HA	1:59:A:GLU:HG3	2	0.18	0.02	0.18
(1,351)	1:148:A:THR:HG21	1:150:A:GLU:H	2	0.18	0.0	0.18
(1,351)	1:148:A:THR:HG22	1:150:A:GLU:H	2	0.18	0.0	0.18
(1,351)	1:148:A:THR:HG23	1:150:A:GLU:H	2	0.18	0.0	0.18
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG11	2	0.17	0.0	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG12	2	0.17	0.0	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG13	2	0.17	0.0	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG11	2	0.17	0.0	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG12	2	0.17	0.0	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG13	2	0.17	0.0	0.17
(1,1344)	1:47:A:ILE:HD11	1:83:A:GLN:HG2	2	0.16	0.06	0.16
(1,1344)	1:47:A:ILE:HD11	1:83:A:GLN:HG3	2	0.16	0.06	0.16
(1,1344)	1:47:A:ILE:HD12	1:83:A:GLN:HG2	2	0.16	0.06	0.16
(1,1344)	1:47:A:ILE:HD12	1:83:A:GLN:HG3	2	0.16	0.06	0.16
(1,1344)	1:47:A:ILE:HD13	1:83:A:GLN:HG2	2	0.16	0.06	0.16
(1,1344)	1:47:A:ILE:HD13	1:83:A:GLN:HG3	2	0.16	0.06	0.16
(1,560)	1:126:A:GLU:HA	1:130:A:ILE:HA	2	0.16	0.02	0.16
(1,794)	1:52:A:THR:HG21	1:58:A:PHE:HD1	2	0.16	0.04	0.16
(1,794)	1:52:A:THR:HG21	1:58:A:PHE:HD2	2	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,794)	1:52:A:THR:HG22	1:58:A:PHE:HD1	2	0.16	0.04	0.16
(1,794)	1:52:A:THR:HG22	1:58:A:PHE:HD2	2	0.16	0.04	0.16
(1,794)	1:52:A:THR:HG23	1:58:A:PHE:HD1	2	0.16	0.04	0.16
(1,794)	1:52:A:THR:HG23	1:58:A:PHE:HD2	2	0.16	0.04	0.16
(1,1182)	1:55:A:GLY:H	1:56:A:VAL:HB	2	0.16	0.04	0.16
(1,169)	1:139:A:GLU:H	1:140:A:GLU:HB2	2	0.16	0.02	0.16
(1,169)	1:139:A:GLU:H	1:140:A:GLU:HB3	2	0.16	0.02	0.16
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG21	2	0.16	0.02	0.16
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG22	2	0.16	0.02	0.16
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG23	2	0.16	0.02	0.16
(1,1228)	1:86:A:VAL:H	1:167:A:LYS:HB2	2	0.16	0.04	0.16
(1,1228)	1:86:A:VAL:H	1:167:A:LYS:HB3	2	0.16	0.04	0.16
(1,1426)	1:83:A:GLN:HE21	1:87:A:GLU:HG2	2	0.16	0.05	0.16
(1,1426)	1:83:A:GLN:HE21	1:87:A:GLU:HG3	2	0.16	0.05	0.16
(1,1426)	1:83:A:GLN:HE22	1:87:A:GLU:HG2	2	0.16	0.05	0.16
(1,1426)	1:83:A:GLN:HE22	1:87:A:GLU:HG3	2	0.16	0.05	0.16
(1,1127)	1:171:A:ASN:H	1:172:A:ILE:HB	2	0.15	0.05	0.15
(1,626)	1:25:A:LEU:HA	1:26:A:VAL:H	2	0.15	0.0	0.15
(1,941)	1:156:A:LYS:HG2	1:160:A:GLU:H	2	0.15	0.03	0.15
(1,941)	1:156:A:LYS:HG3	1:160:A:GLU:H	2	0.15	0.03	0.15
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG21	2	0.15	0.03	0.15
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG22	2	0.15	0.03	0.15
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG23	2	0.15	0.03	0.15
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG21	2	0.15	0.03	0.15
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG22	2	0.15	0.03	0.15
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG23	2	0.15	0.03	0.15
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB1	2	0.15	0.0	0.15
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB2	2	0.15	0.0	0.15
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB3	2	0.15	0.0	0.15
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB1	2	0.15	0.0	0.15
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB2	2	0.15	0.0	0.15
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB3	2	0.15	0.0	0.15
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB1	2	0.15	0.02	0.15
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB2	2	0.15	0.02	0.15
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB3	2	0.15	0.02	0.15
(1,528)	1:114:A:MET:HE1	1:118:A:MET:HG2	2	0.14	0.03	0.14
(1,528)	1:114:A:MET:HE1	1:118:A:MET:HG3	2	0.14	0.03	0.14
(1,528)	1:114:A:MET:HE2	1:118:A:MET:HG2	2	0.14	0.03	0.14
(1,528)	1:114:A:MET:HE2	1:118:A:MET:HG3	2	0.14	0.03	0.14
(1,528)	1:114:A:MET:HE3	1:118:A:MET:HG2	2	0.14	0.03	0.14
(1,528)	1:114:A:MET:HE3	1:118:A:MET:HG3	2	0.14	0.03	0.14
(1,132)	1:49:A:LYS:HB2	1:52:A:THR:HB	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,132)	1:49:A:LYS:HB3	1:52:A:THR:HB	2	0.14	0.02	0.14
(1,154)	1:81:A:LYS:HD2	1:128:A:VAL:HB	2	0.14	0.02	0.14
(1,154)	1:81:A:LYS:HD3	1:128:A:VAL:HB	2	0.14	0.02	0.14
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD21	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD22	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD23	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD21	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD22	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD23	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD21	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD22	2	0.14	0.01	0.14
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD23	2	0.14	0.01	0.14
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG11	2	0.14	0.01	0.14
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG12	2	0.14	0.01	0.14
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG13	2	0.14	0.01	0.14
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD11	2	0.14	0.02	0.14
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD12	2	0.14	0.02	0.14
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD13	2	0.14	0.02	0.14
(1,679)	1:29:A:THR:HA	1:30:A:ASN:HA	2	0.14	0.02	0.14
(1,712)	1:41:A:LYS:H	1:41:A:LYS:HD2	2	0.14	0.02	0.14
(1,712)	1:41:A:LYS:H	1:41:A:LYS:HD3	2	0.14	0.02	0.14
(1,1272)	1:34:A:GLU:H	1:34:A:GLU:HG2	2	0.14	0.01	0.14
(1,1272)	1:34:A:GLU:H	1:34:A:GLU:HG3	2	0.14	0.01	0.14
(1,699)	1:45:A:LEU:HG	1:46:A:LYS:HA	2	0.13	0.01	0.13
(1,1129)	1:101:A:LYS:HD2	1:102:A:LEU:H	2	0.12	0.02	0.12
(1,1129)	1:101:A:LYS:HD3	1:102:A:LEU:H	2	0.12	0.02	0.12
(1,1562)	1:122:A:VAL:HG11	1:134:A:LYS:HB2	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG11	1:134:A:LYS:HB3	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG12	1:134:A:LYS:HB2	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG12	1:134:A:LYS:HB3	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG13	1:134:A:LYS:HB2	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG13	1:134:A:LYS:HB3	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG21	1:134:A:LYS:HB2	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG21	1:134:A:LYS:HB3	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG22	1:134:A:LYS:HB2	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG22	1:134:A:LYS:HB3	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG23	1:134:A:LYS:HB2	2	0.12	0.01	0.12
(1,1562)	1:122:A:VAL:HG23	1:134:A:LYS:HB3	2	0.12	0.01	0.12
(1,1591)	1:133:A:LEU:HD11	1:163:A:LEU:HA	2	0.12	0.02	0.12
(1,1591)	1:133:A:LEU:HD12	1:163:A:LEU:HA	2	0.12	0.02	0.12
(1,1591)	1:133:A:LEU:HD13	1:163:A:LEU:HA	2	0.12	0.02	0.12
(1,1591)	1:133:A:LEU:HD21	1:163:A:LEU:HA	2	0.12	0.02	0.12

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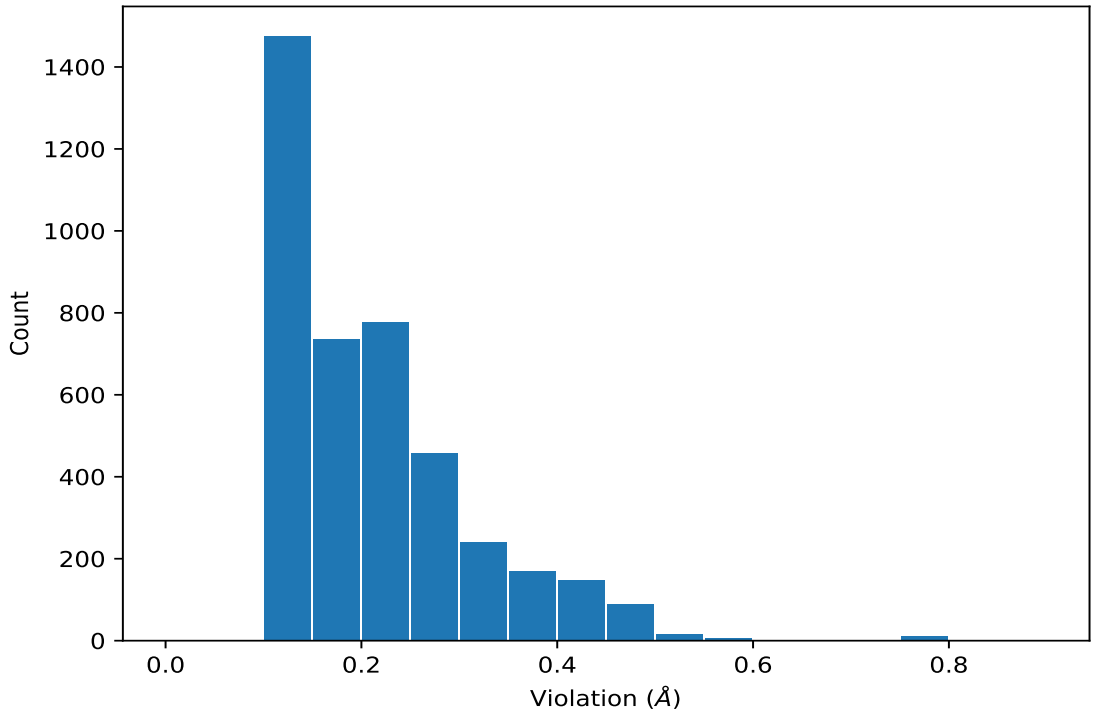
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1591)	1:133:A:LEU:HD22	1:163:A:LEU:HA	2	0.12	0.02	0.12
(1,1591)	1:133:A:LEU:HD23	1:163:A:LEU:HA	2	0.12	0.02	0.12
(1,673)	1:80:A:ALA:HA	1:83:A:GLN:HB3	2	0.12	0.02	0.12
(1,1490)	1:102:A:LEU:HD11	1:110:A:GLN:HE21	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD11	1:110:A:GLN:HE22	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD12	1:110:A:GLN:HE21	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD12	1:110:A:GLN:HE22	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD13	1:110:A:GLN:HE21	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD13	1:110:A:GLN:HE22	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD21	1:110:A:GLN:HE21	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD21	1:110:A:GLN:HE22	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD22	1:110:A:GLN:HE21	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD22	1:110:A:GLN:HE22	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD23	1:110:A:GLN:HE21	2	0.12	0.01	0.12
(1,1490)	1:102:A:LEU:HD23	1:110:A:GLN:HE22	2	0.12	0.01	0.12
(1,155)	1:51:A:ALA:HB1	1:56:A:VAL:HB	2	0.12	0.02	0.12
(1,155)	1:51:A:ALA:HB2	1:56:A:VAL:HB	2	0.12	0.02	0.12
(1,155)	1:51:A:ALA:HB3	1:56:A:VAL:HB	2	0.12	0.02	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD11	2	0.12	0.0	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD12	2	0.12	0.0	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD13	2	0.12	0.0	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD21	2	0.12	0.0	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD22	2	0.12	0.0	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD23	2	0.12	0.0	0.12
(1,225)	1:77:A:LEU:HG	1:81:A:LYS:HG2	2	0.11	0.0	0.11
(1,225)	1:77:A:LEU:HG	1:81:A:LYS:HG3	2	0.11	0.0	0.11
(1,181)	1:41:A:LYS:HD2	1:120:A:GLU:HB2	2	0.11	0.0	0.11
(1,181)	1:41:A:LYS:HD2	1:120:A:GLU:HB3	2	0.11	0.0	0.11
(1,181)	1:41:A:LYS:HD3	1:120:A:GLU:HB2	2	0.11	0.0	0.11
(1,181)	1:41:A:LYS:HD3	1:120:A:GLU:HB3	2	0.11	0.0	0.11

[1]Number of violated models, [2]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)
(1,9)	1:151:A:ARG:HD2	1:152:A:LEU:HA	6	0.87
(1,9)	1:151:A:ARG:HD3	1:152:A:LEU:HA	6	0.87
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	10	0.79
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	10	0.79
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	10	0.79
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	10	0.79
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	10	0.79
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	10	0.79
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	7	0.79
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	7	0.79
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	7	0.79
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	7	0.79
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	7	0.79
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	7	0.79
(1,739)	1:131:A:ILE:HB	1:132:A:GLY:HA3	2	0.62
(1,100)	1:83:A:GLN:H	1:83:A:GLN:HG2	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:158:A:GLN:H	1:158:A:GLN:HG2	9	0.57
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB2	8	0.55
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB3	8	0.55
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB2	8	0.55
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB3	8	0.55
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD11	5	0.54
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD12	5	0.54
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD13	5	0.54
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD11	5	0.54
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD12	5	0.54
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD13	5	0.54
(1,618)	1:146:A:ILE:HG21	1:152:A:LEU:HA	3	0.52
(1,618)	1:146:A:ILE:HG22	1:152:A:LEU:HA	3	0.52
(1,618)	1:146:A:ILE:HG23	1:152:A:LEU:HA	3	0.52
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	5	0.5
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	5	0.5
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	5	0.5
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	5	0.5
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	5	0.5
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	5	0.5
(1,1151)	1:141:A:SER:H	1:146:A:ILE:HB	2	0.5
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD11	9	0.49
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD12	9	0.49
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD13	9	0.49
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD21	9	0.49
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD22	9	0.49
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD23	9	0.49
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB2	9	0.49
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB3	9	0.49
(1,1309)	1:40:A:LEU:HD11	1:121:A:VAL:HB	8	0.49
(1,1309)	1:40:A:LEU:HD12	1:121:A:VAL:HB	8	0.49
(1,1309)	1:40:A:LEU:HD13	1:121:A:VAL:HB	8	0.49
(1,1309)	1:40:A:LEU:HD21	1:121:A:VAL:HB	8	0.49
(1,1309)	1:40:A:LEU:HD22	1:121:A:VAL:HB	8	0.49
(1,1309)	1:40:A:LEU:HD23	1:121:A:VAL:HB	8	0.49
(1,739)	1:131:A:ILE:HB	1:132:A:GLY:HA3	3	0.49
(1,694)	1:114:A:MET:HE1	1:118:A:MET:HB3	10	0.49
(1,694)	1:114:A:MET:HE2	1:118:A:MET:HB3	10	0.49
(1,694)	1:114:A:MET:HE3	1:118:A:MET:HB3	10	0.49
(1,101)	1:83:A:GLN:H	1:83:A:GLN:HG3	4	0.49
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	4	0.47
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	4	0.47
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	4	0.47
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	4	0.47
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	4	0.47
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD11	9	0.46
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD12	9	0.46
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD13	9	0.46
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD11	9	0.46
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD12	9	0.46
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD13	9	0.46
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	8	0.46
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	8	0.46
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	8	0.46
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	8	0.46
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	8	0.46
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	8	0.46
(1,1564)	1:122:A:VAL:HG11	1:134:A:LYS:HE2	10	0.46
(1,1564)	1:122:A:VAL:HG11	1:134:A:LYS:HE3	10	0.46
(1,1564)	1:122:A:VAL:HG12	1:134:A:LYS:HE2	10	0.46
(1,1564)	1:122:A:VAL:HG12	1:134:A:LYS:HE3	10	0.46
(1,1564)	1:122:A:VAL:HG13	1:134:A:LYS:HE2	10	0.46
(1,1564)	1:122:A:VAL:HG13	1:134:A:LYS:HE3	10	0.46
(1,1564)	1:122:A:VAL:HG21	1:134:A:LYS:HE2	10	0.46
(1,1564)	1:122:A:VAL:HG21	1:134:A:LYS:HE3	10	0.46
(1,1564)	1:122:A:VAL:HG22	1:134:A:LYS:HE2	10	0.46
(1,1564)	1:122:A:VAL:HG22	1:134:A:LYS:HE3	10	0.46
(1,1564)	1:122:A:VAL:HG23	1:134:A:LYS:HE2	10	0.46
(1,1564)	1:122:A:VAL:HG23	1:134:A:LYS:HE3	10	0.46
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	3	0.46
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	3	0.46
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG11	7	0.46
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG12	7	0.46
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG13	7	0.46
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG21	7	0.46
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG22	7	0.46
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG23	7	0.46
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG11	7	0.46
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG12	7	0.46
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG13	7	0.46
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG21	7	0.46
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG22	7	0.46
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG23	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB2	8	0.46
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB3	8	0.46
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB2	4	0.45
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB3	4	0.45
(1,1116)	1:101:A:LYS:HD2	1:104:A:GLU:H	1	0.45
(1,1116)	1:101:A:LYS:HD3	1:104:A:GLU:H	1	0.45
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	9	0.45
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	9	0.45
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB1	9	0.45
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB2	9	0.45
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB3	9	0.45
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB1	9	0.45
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB2	9	0.45
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB3	9	0.45
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	3	0.45
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	3	0.45
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	3	0.45
(1,301)	1:45:A:LEU:HA	1:45:A:LEU:HD21	2	0.45
(1,301)	1:45:A:LEU:HA	1:45:A:LEU:HD22	2	0.45
(1,301)	1:45:A:LEU:HA	1:45:A:LEU:HD23	2	0.45
(1,191)	1:152:A:LEU:HD21	1:154:A:ALA:H	3	0.45
(1,191)	1:152:A:LEU:HD22	1:154:A:ALA:H	3	0.45
(1,191)	1:152:A:LEU:HD23	1:154:A:ALA:H	3	0.45
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	8	0.45
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	8	0.45
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG21	2	0.44
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG22	2	0.44
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG23	2	0.44
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG21	2	0.44
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG22	2	0.44
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG23	2	0.44
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG21	2	0.44
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG22	2	0.44
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG23	2	0.44
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG21	2	0.44
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG22	2	0.44
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG23	2	0.44
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG21	2	0.44
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG22	2	0.44
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG23	2	0.44
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG21	2	0.44
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG22	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG23	2	0.44
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB2	3	0.44
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB3	3	0.44
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB2	3	0.44
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB3	3	0.44
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB2	3	0.44
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB3	3	0.44
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB2	3	0.44
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB3	3	0.44
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB2	3	0.44
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB3	3	0.44
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB2	3	0.44
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB3	3	0.44
(1,1376)	1:60:A:ALA:HA	1:64:A:LEU:HB2	2	0.44
(1,1376)	1:60:A:ALA:HA	1:64:A:LEU:HB3	2	0.44
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG21	3	0.44
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG22	3	0.44
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG23	3	0.44
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG21	3	0.44
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG22	3	0.44
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG23	3	0.44
(1,782)	1:91:A:PHE:HA	1:94:A:ILE:HB	3	0.44
(1,739)	1:131:A:ILE:HB	1:132:A:GLY:HA3	1	0.44
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	4	0.44
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	4	0.44
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	5	0.43
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	5	0.43
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	5	0.43
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	5	0.43
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	5	0.43
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	5	0.43
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG11	2	0.43
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG12	2	0.43
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG13	2	0.43
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG21	2	0.43
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG22	2	0.43
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG23	2	0.43
(1,1048)	1:37:A:SER:H	1:41:A:LYS:HD2	4	0.43
(1,1048)	1:37:A:SER:H	1:41:A:LYS:HD3	4	0.43
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	5	0.43
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	8	0.43
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	9	0.43
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	9	0.43
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	9	0.43
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	9	0.43
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	9	0.43
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	9	0.43
(1,643)	1:54:A:LYS:HA	1:54:A:LYS:HD2	9	0.43
(1,643)	1:54:A:LYS:HA	1:54:A:LYS:HD3	9	0.43
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	1	0.43
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	1	0.43
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	1	0.43
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	7	0.43
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	2	0.43
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	2	0.43
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	5	0.43
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	5	0.43
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	9	0.43
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	9	0.43
(1,18)	1:25:A:LEU:HB2	1:26:A:VAL:HA	9	0.43
(1,1611)	1:137:A:VAL:HB	1:138:A:LEU:HD11	10	0.42
(1,1611)	1:137:A:VAL:HB	1:138:A:LEU:HD12	10	0.42
(1,1611)	1:137:A:VAL:HB	1:138:A:LEU:HD13	10	0.42
(1,1611)	1:137:A:VAL:HB	1:138:A:LEU:HD21	10	0.42
(1,1611)	1:137:A:VAL:HB	1:138:A:LEU:HD22	10	0.42
(1,1611)	1:137:A:VAL:HB	1:138:A:LEU:HD23	10	0.42
(1,1571)	1:128:A:VAL:HG21	1:129:A:GLY:HA2	1	0.42
(1,1571)	1:128:A:VAL:HG21	1:129:A:GLY:HA3	1	0.42
(1,1571)	1:128:A:VAL:HG22	1:129:A:GLY:HA2	1	0.42
(1,1571)	1:128:A:VAL:HG22	1:129:A:GLY:HA3	1	0.42
(1,1571)	1:128:A:VAL:HG23	1:129:A:GLY:HA2	1	0.42
(1,1571)	1:128:A:VAL:HG23	1:129:A:GLY:HA3	1	0.42
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB2	9	0.42
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB3	9	0.42
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB2	9	0.42
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB3	9	0.42
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB2	9	0.42
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB3	9	0.42
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB2	9	0.42
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB3	9	0.42
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB2	9	0.42
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB3	9	0.42
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB2	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB3	9	0.42
(1,1293)	1:40:A:LEU:HD11	1:41:A:LYS:HA	9	0.42
(1,1293)	1:40:A:LEU:HD12	1:41:A:LYS:HA	9	0.42
(1,1293)	1:40:A:LEU:HD13	1:41:A:LYS:HA	9	0.42
(1,1293)	1:40:A:LEU:HD21	1:41:A:LYS:HA	9	0.42
(1,1293)	1:40:A:LEU:HD22	1:41:A:LYS:HA	9	0.42
(1,1293)	1:40:A:LEU:HD23	1:41:A:LYS:HA	9	0.42
(1,1012)	1:148:A:THR:H	1:151:A:ARG:H	3	0.42
(1,643)	1:54:A:LYS:HA	1:54:A:LYS:HD2	7	0.42
(1,643)	1:54:A:LYS:HA	1:54:A:LYS:HD3	7	0.42
(1,134)	1:44:A:ILE:HA	1:48:A:LYS:HB2	10	0.42
(1,134)	1:44:A:ILE:HA	1:48:A:LYS:HB3	10	0.42
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	4	0.41
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	4	0.41
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	4	0.41
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	4	0.41
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	4	0.41
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	4	0.41
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	4	0.41
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	4	0.41
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	4	0.41
(1,164)	1:184:A:LYS:H	1:184:A:LYS:HD2	3	0.41
(1,164)	1:184:A:LYS:H	1:184:A:LYS:HD3	3	0.41
(1,1520)	1:114:A:MET:H	1:152:A:LEU:HD11	9	0.4
(1,1520)	1:114:A:MET:H	1:152:A:LEU:HD12	9	0.4
(1,1520)	1:114:A:MET:H	1:152:A:LEU:HD13	9	0.4
(1,1520)	1:114:A:MET:H	1:152:A:LEU:HD21	9	0.4
(1,1520)	1:114:A:MET:H	1:152:A:LEU:HD22	9	0.4
(1,1520)	1:114:A:MET:H	1:152:A:LEU:HD23	9	0.4
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE2	3	0.4
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE3	3	0.4
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE2	3	0.4
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE3	3	0.4
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE2	3	0.4
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE3	3	0.4
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE2	3	0.4
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE3	3	0.4
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE2	3	0.4
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE3	3	0.4
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE2	3	0.4
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE3	3	0.4
(1,1219)	1:146:A:ILE:HD11	1:149:A:ALA:H	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:146:A:ILE:HD12	1:149:A:ALA:H	7	0.4
(1,1219)	1:146:A:ILE:HD13	1:149:A:ALA:H	7	0.4
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG11	1	0.4
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG12	1	0.4
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG13	1	0.4
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	4	0.39
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	4	0.39
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	7	0.39
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	7	0.39
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	7	0.39
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	7	0.39
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	7	0.39
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	7	0.39
(1,1168)	1:102:A:LEU:HD21	1:106:A:GLY:H	2	0.39
(1,1168)	1:102:A:LEU:HD22	1:106:A:GLY:H	2	0.39
(1,1168)	1:102:A:LEU:HD23	1:106:A:GLY:H	2	0.39
(1,542)	1:38:A:LYS:HA	1:38:A:LYS:HE2	7	0.39
(1,542)	1:38:A:LYS:HA	1:38:A:LYS:HE3	7	0.39
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	8	0.39
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	8	0.39
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	8	0.39
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	2	0.39
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	2	0.39
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	2	0.39
(1,151)	1:134:A:LYS:HA	1:137:A:VAL:HB	10	0.39
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	4	0.39
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	4	0.39
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	4	0.39
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	4	0.39
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	4	0.39
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	4	0.39
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	1	0.38
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	1	0.38
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	1	0.38
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	1	0.38
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	1	0.38
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	1	0.38
(1,1385)	1:64:A:LEU:HD11	1:67:A:GLY:HA2	6	0.38
(1,1385)	1:64:A:LEU:HD11	1:67:A:GLY:HA3	6	0.38
(1,1385)	1:64:A:LEU:HD12	1:67:A:GLY:HA2	6	0.38
(1,1385)	1:64:A:LEU:HD12	1:67:A:GLY:HA3	6	0.38
(1,1385)	1:64:A:LEU:HD13	1:67:A:GLY:HA2	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:64:A:LEU:HD13	1:67:A:GLY:HA3	6	0.38
(1,1385)	1:64:A:LEU:HD21	1:67:A:GLY:HA2	6	0.38
(1,1385)	1:64:A:LEU:HD21	1:67:A:GLY:HA3	6	0.38
(1,1385)	1:64:A:LEU:HD22	1:67:A:GLY:HA2	6	0.38
(1,1385)	1:64:A:LEU:HD22	1:67:A:GLY:HA3	6	0.38
(1,1385)	1:64:A:LEU:HD23	1:67:A:GLY:HA2	6	0.38
(1,1385)	1:64:A:LEU:HD23	1:67:A:GLY:HA3	6	0.38
(1,1151)	1:141:A:SER:H	1:146:A:ILE:HB	10	0.38
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	4	0.38
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	4	0.38
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	4	0.38
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	8	0.38
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	8	0.38
(1,742)	1:131:A:ILE:HD11	1:132:A:GLY:H	2	0.38
(1,742)	1:131:A:ILE:HD12	1:132:A:GLY:H	2	0.38
(1,742)	1:131:A:ILE:HD13	1:132:A:GLY:H	2	0.38
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG2	7	0.38
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG3	7	0.38
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG2	7	0.38
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG3	7	0.38
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG2	7	0.38
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG3	7	0.38
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	5	0.38
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	5	0.38
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	5	0.38
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	8	0.38
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	8	0.38
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	8	0.38
(1,237)	1:133:A:LEU:HD21	1:162:A:GLN:H	4	0.38
(1,237)	1:133:A:LEU:HD22	1:162:A:GLN:H	4	0.38
(1,237)	1:133:A:LEU:HD23	1:162:A:GLN:H	4	0.38
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	10	0.38
(1,1398)	1:70:A:VAL:HG11	1:72:A:SER:HA	4	0.37
(1,1398)	1:70:A:VAL:HG12	1:72:A:SER:HA	4	0.37
(1,1398)	1:70:A:VAL:HG13	1:72:A:SER:HA	4	0.37
(1,1398)	1:70:A:VAL:HG21	1:72:A:SER:HA	4	0.37
(1,1398)	1:70:A:VAL:HG22	1:72:A:SER:HA	4	0.37
(1,1398)	1:70:A:VAL:HG23	1:72:A:SER:HA	4	0.37
(1,1385)	1:64:A:LEU:HD11	1:67:A:GLY:HA2	8	0.37
(1,1385)	1:64:A:LEU:HD11	1:67:A:GLY:HA3	8	0.37
(1,1385)	1:64:A:LEU:HD12	1:67:A:GLY:HA2	8	0.37
(1,1385)	1:64:A:LEU:HD12	1:67:A:GLY:HA3	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1385)	1:64:A:LEU:HD13	1:67:A:GLY:HA2	8	0.37
(1,1385)	1:64:A:LEU:HD13	1:67:A:GLY:HA3	8	0.37
(1,1385)	1:64:A:LEU:HD21	1:67:A:GLY:HA2	8	0.37
(1,1385)	1:64:A:LEU:HD21	1:67:A:GLY:HA3	8	0.37
(1,1385)	1:64:A:LEU:HD22	1:67:A:GLY:HA2	8	0.37
(1,1385)	1:64:A:LEU:HD22	1:67:A:GLY:HA3	8	0.37
(1,1385)	1:64:A:LEU:HD23	1:67:A:GLY:HA2	8	0.37
(1,1385)	1:64:A:LEU:HD23	1:67:A:GLY:HA3	8	0.37
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	2	0.37
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	2	0.37
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	2	0.37
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	2	0.37
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	2	0.37
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	2	0.37
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	2	0.37
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	2	0.37
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	2	0.37
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	2	0.37
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	2	0.37
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	2	0.37
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD11	9	0.37
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD12	9	0.37
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD13	9	0.37
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD21	9	0.37
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD22	9	0.37
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD23	9	0.37
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	7	0.37
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	7	0.37
(1,542)	1:38:A:LYS:HA	1:38:A:LYS:HE2	2	0.37
(1,542)	1:38:A:LYS:HA	1:38:A:LYS:HE3	2	0.37
(1,523)	1:44:A:ILE:HG21	1:125:A:LEU:HA	9	0.37
(1,523)	1:44:A:ILE:HG22	1:125:A:LEU:HA	9	0.37
(1,523)	1:44:A:ILE:HG23	1:125:A:LEU:HA	9	0.37
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG21	9	0.37
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG22	9	0.37
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG23	9	0.37
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	4	0.37
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	4	0.37
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	4	0.37
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE2	8	0.37
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE3	8	0.37
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE2	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE3	8	0.37
(1,1571)	1:128:A:VAL:HG21	1:129:A:GLY:HA2	6	0.36
(1,1571)	1:128:A:VAL:HG21	1:129:A:GLY:HA3	6	0.36
(1,1571)	1:128:A:VAL:HG22	1:129:A:GLY:HA2	6	0.36
(1,1571)	1:128:A:VAL:HG22	1:129:A:GLY:HA3	6	0.36
(1,1571)	1:128:A:VAL:HG23	1:129:A:GLY:HA2	6	0.36
(1,1571)	1:128:A:VAL:HG23	1:129:A:GLY:HA3	6	0.36
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG2	9	0.36
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG3	9	0.36
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG2	9	0.36
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG3	9	0.36
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG2	9	0.36
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG3	9	0.36
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG2	9	0.36
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG3	9	0.36
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG2	9	0.36
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG3	9	0.36
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG2	9	0.36
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG3	9	0.36
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	5	0.36
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	5	0.36
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	5	0.36
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD11	8	0.36
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD12	8	0.36
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD13	8	0.36
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA2	3	0.36
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA3	3	0.36
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA2	3	0.36
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA3	3	0.36
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA2	3	0.36
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA3	3	0.36
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB1	7	0.36
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB2	7	0.36
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB3	7	0.36
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB1	7	0.36
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB2	7	0.36
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB3	7	0.36
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB1	7	0.36
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB2	7	0.36
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB3	7	0.36
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG11	6	0.36
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG12	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:127:A:ASP:H	1:128:A:VAL:HG13	6	0.36
(1,318)	1:102:A:LEU:HD11	1:106:A:GLY:H	6	0.36
(1,318)	1:102:A:LEU:HD12	1:106:A:GLY:H	6	0.36
(1,318)	1:102:A:LEU:HD13	1:106:A:GLY:H	6	0.36
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	1	0.36
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	1	0.36
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	1	0.36
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB2	2	0.35
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB3	2	0.35
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB2	6	0.35
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB3	6	0.35
(1,1219)	1:146:A:ILE:HD11	1:149:A:ALA:H	1	0.35
(1,1219)	1:146:A:ILE:HD12	1:149:A:ALA:H	1	0.35
(1,1219)	1:146:A:ILE:HD13	1:149:A:ALA:H	1	0.35
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD11	3	0.35
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD12	3	0.35
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD13	3	0.35
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	1	0.35
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	1	0.35
(1,662)	1:146:A:ILE:HD11	1:155:A:ALA:H	3	0.35
(1,662)	1:146:A:ILE:HD12	1:155:A:ALA:H	3	0.35
(1,662)	1:146:A:ILE:HD13	1:155:A:ALA:H	3	0.35
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	10	0.35
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	10	0.35
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	10	0.35
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	10	0.35
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	10	0.35
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	10	0.35
(1,42)	1:37:A:SER:HA	1:39:A:ASP:HB3	3	0.35
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	7	0.34
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	7	0.34
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	7	0.34
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	7	0.34
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	7	0.34
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	7	0.34
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	7	0.34
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	7	0.34
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	7	0.34
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	7	0.34
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	7	0.34
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	7	0.34
(1,1333)	1:44:A:ILE:HG12	1:48:A:LYS:H	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1333)	1:44:A:ILE:HG13	1:48:A:LYS:H	7	0.34
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB2	3	0.34
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB3	3	0.34
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB2	3	0.34
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB3	3	0.34
(1,1195)	1:111:A:PHE:H	1:147:A:ASN:HA	8	0.34
(1,1151)	1:141:A:SER:H	1:146:A:ILE:HB	1	0.34
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	1	0.34
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	1	0.34
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	1	0.34
(1,950)	1:112:A:LEU:HG	1:115:A:PHE:H	5	0.34
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	2	0.34
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD21	2	0.34
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD22	2	0.34
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD23	2	0.34
(1,191)	1:152:A:LEU:HD21	1:154:A:ALA:H	5	0.34
(1,191)	1:152:A:LEU:HD22	1:154:A:ALA:H	5	0.34
(1,191)	1:152:A:LEU:HD23	1:154:A:ALA:H	5	0.34
(1,186)	1:172:A:ILE:HG21	1:173:A:GLU:HB2	9	0.34
(1,186)	1:172:A:ILE:HG21	1:173:A:GLU:HB3	9	0.34
(1,186)	1:172:A:ILE:HG22	1:173:A:GLU:HB2	9	0.34
(1,186)	1:172:A:ILE:HG22	1:173:A:GLU:HB3	9	0.34
(1,186)	1:172:A:ILE:HG23	1:173:A:GLU:HB2	9	0.34
(1,186)	1:172:A:ILE:HG23	1:173:A:GLU:HB3	9	0.34
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB2	8	0.34
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB3	8	0.34
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG2	9	0.33
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG3	9	0.33
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG2	9	0.33
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG3	9	0.33
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG2	9	0.33
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG3	9	0.33
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG2	4	0.33
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG3	4	0.33
(1,1517)	1:112:A:LEU:HD11	1:147:A:ASN:HA	5	0.33
(1,1517)	1:112:A:LEU:HD12	1:147:A:ASN:HA	5	0.33
(1,1517)	1:112:A:LEU:HD13	1:147:A:ASN:HA	5	0.33
(1,1517)	1:112:A:LEU:HD21	1:147:A:ASN:HA	5	0.33
(1,1517)	1:112:A:LEU:HD22	1:147:A:ASN:HA	5	0.33
(1,1517)	1:112:A:LEU:HD23	1:147:A:ASN:HA	5	0.33
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB2	3	0.33
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB3	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1275)	1:34:A:GLU:HB2	1:35:A:SER:HB2	2	0.33
(1,1275)	1:34:A:GLU:HB2	1:35:A:SER:HB3	2	0.33
(1,1275)	1:34:A:GLU:HB3	1:35:A:SER:HB2	2	0.33
(1,1275)	1:34:A:GLU:HB3	1:35:A:SER:HB3	2	0.33
(1,1208)	1:64:A:LEU:HD11	1:67:A:GLY:H	7	0.33
(1,1208)	1:64:A:LEU:HD12	1:67:A:GLY:H	7	0.33
(1,1208)	1:64:A:LEU:HD13	1:67:A:GLY:H	7	0.33
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	7	0.33
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	7	0.33
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	7	0.33
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	10	0.33
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	10	0.33
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	10	0.33
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	10	0.33
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	10	0.33
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG21	6	0.33
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG22	6	0.33
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG23	6	0.33
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG21	6	0.33
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG22	6	0.33
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG23	6	0.33
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	3	0.33
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG2	1	0.33
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG3	1	0.33
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	6	0.32
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	6	0.32
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	6	0.32
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	6	0.32
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	6	0.32
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	6	0.32
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	4	0.32
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	4	0.32
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD11	4	0.32
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD12	4	0.32
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD13	4	0.32
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD21	4	0.32
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD22	4	0.32
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD23	4	0.32
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD11	4	0.32
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD12	4	0.32
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD13	4	0.32
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD21	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD22	4	0.32
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD23	4	0.32
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD11	7	0.32
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD12	7	0.32
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD13	7	0.32
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD21	7	0.32
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD22	7	0.32
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD23	7	0.32
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD11	7	0.32
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD12	7	0.32
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD13	7	0.32
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD21	7	0.32
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD22	7	0.32
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD23	7	0.32
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD11	3	0.32
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD12	3	0.32
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD13	3	0.32
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD21	3	0.32
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD22	3	0.32
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD23	3	0.32
(1,1219)	1:146:A:ILE:HD11	1:149:A:ALA:H	5	0.32
(1,1219)	1:146:A:ILE:HD12	1:149:A:ALA:H	5	0.32
(1,1219)	1:146:A:ILE:HD13	1:149:A:ALA:H	5	0.32
(1,1042)	1:121:A:VAL:HB	1:124:A:SER:H	4	0.32
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	3	0.32
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	3	0.32
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	4	0.32
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	4	0.32
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	6	0.32
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	6	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	3	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	3	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	3	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	3	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	3	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	3	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	5	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	5	0.32
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	5	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	5	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	5	0.32
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:131:A:ILE:HD11	1:132:A:GLY:H	7	0.32
(1,742)	1:131:A:ILE:HD12	1:132:A:GLY:H	7	0.32
(1,742)	1:131:A:ILE:HD13	1:132:A:GLY:H	7	0.32
(1,739)	1:131:A:ILE:HB	1:132:A:GLY:HA3	8	0.32
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	9	0.32
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	9	0.32
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	9	0.32
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	9	0.32
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	9	0.32
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	9	0.32
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	9	0.32
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD21	10	0.32
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD22	10	0.32
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD23	10	0.32
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG2	4	0.32
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG3	4	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG2	1	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG3	1	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG2	3	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG3	3	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG2	6	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG3	6	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG2	10	0.32
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG3	10	0.32
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG21	6	0.31
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG22	6	0.31
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG23	6	0.31
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG21	6	0.31
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG22	6	0.31
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG23	6	0.31
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG21	6	0.31
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG22	6	0.31
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG23	6	0.31
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG21	6	0.31
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG22	6	0.31
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG23	6	0.31
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG21	6	0.31
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG22	6	0.31
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG23	6	0.31
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG21	6	0.31
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG22	6	0.31
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG23	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD11	2	0.31
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD12	2	0.31
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD13	2	0.31
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD21	2	0.31
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD22	2	0.31
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD23	2	0.31
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	10	0.31
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	10	0.31
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	10	0.31
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	10	0.31
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	10	0.31
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	10	0.31
(1,1233)	1:89:A:GLY:H	1:90:A:LYS:HD2	7	0.31
(1,1233)	1:89:A:GLY:H	1:90:A:LYS:HD3	7	0.31
(1,739)	1:131:A:ILE:HB	1:132:A:GLY:HA3	7	0.31
(1,709)	1:65:A:LYS:H	1:65:A:LYS:HD2	1	0.31
(1,709)	1:65:A:LYS:H	1:65:A:LYS:HD3	1	0.31
(1,617)	1:116:A:ASP:HA	1:119:A:LEU:HD11	5	0.31
(1,617)	1:116:A:ASP:HA	1:119:A:LEU:HD12	5	0.31
(1,617)	1:116:A:ASP:HA	1:119:A:LEU:HD13	5	0.31
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	8	0.31
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	8	0.31
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	8	0.31
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	8	0.31
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	8	0.31
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	8	0.31
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	8	0.31
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	8	0.31
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	8	0.31
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	8	0.31
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	6	0.31
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	6	0.31
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	6	0.31
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	5	0.31
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB2	5	0.31
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB3	5	0.31
(1,18)	1:25:A:LEU:HB2	1:26:A:VAL:HA	10	0.31
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	3	0.3
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	3	0.3
(1,1511)	1:112:A:LEU:HB2	1:116:A:ASP:H	3	0.3
(1,1511)	1:112:A:LEU:HB3	1:116:A:ASP:H	3	0.3
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	10	0.3
(1,1458)	1:92:A:LEU:HD11	1:160:A:GLU:HG2	10	0.3
(1,1458)	1:92:A:LEU:HD11	1:160:A:GLU:HG3	10	0.3
(1,1458)	1:92:A:LEU:HD12	1:160:A:GLU:HG2	10	0.3
(1,1458)	1:92:A:LEU:HD12	1:160:A:GLU:HG3	10	0.3
(1,1458)	1:92:A:LEU:HD13	1:160:A:GLU:HG2	10	0.3
(1,1458)	1:92:A:LEU:HD13	1:160:A:GLU:HG3	10	0.3
(1,1458)	1:92:A:LEU:HD21	1:160:A:GLU:HG2	10	0.3
(1,1458)	1:92:A:LEU:HD21	1:160:A:GLU:HG3	10	0.3
(1,1458)	1:92:A:LEU:HD22	1:160:A:GLU:HG2	10	0.3
(1,1458)	1:92:A:LEU:HD22	1:160:A:GLU:HG3	10	0.3
(1,1458)	1:92:A:LEU:HD23	1:160:A:GLU:HG2	10	0.3
(1,1458)	1:92:A:LEU:HD23	1:160:A:GLU:HG3	10	0.3
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	7	0.3
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	7	0.3
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	7	0.3
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	7	0.3
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	7	0.3
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	7	0.3
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	7	0.3
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	7	0.3
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	7	0.3
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	7	0.3
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	7	0.3
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	7	0.3
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB2	5	0.3
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB3	5	0.3
(1,1233)	1:89:A:GLY:H	1:90:A:LYS:HD2	9	0.3
(1,1233)	1:89:A:GLY:H	1:90:A:LYS:HD3	9	0.3
(1,1210)	1:40:A:LEU:H	1:44:A:ILE:HD11	7	0.3
(1,1210)	1:40:A:LEU:H	1:44:A:ILE:HD12	7	0.3
(1,1210)	1:40:A:LEU:H	1:44:A:ILE:HD13	7	0.3
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	5	0.3
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	5	0.3
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	5	0.3
(1,1041)	1:159:A:ILE:HB	1:162:A:GLN:H	6	0.3
(1,1012)	1:148:A:THR:H	1:151:A:ARG:H	10	0.3
(1,739)	1:131:A:ILE:HB	1:132:A:GLY:HA3	4	0.3
(1,669)	1:113:A:ALA:HA	1:116:A:ASP:HB3	5	0.3
(1,663)	1:146:A:ILE:HD11	1:147:A:ASN:H	9	0.3
(1,663)	1:146:A:ILE:HD12	1:147:A:ASN:H	9	0.3
(1,663)	1:146:A:ILE:HD13	1:147:A:ASN:H	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD11	2	0.3
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD12	2	0.3
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD13	2	0.3
(1,557)	1:82:A:VAL:H	1:85:A:ILE:HD11	10	0.3
(1,557)	1:82:A:VAL:H	1:85:A:ILE:HD12	10	0.3
(1,557)	1:82:A:VAL:H	1:85:A:ILE:HD13	10	0.3
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	8	0.3
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	8	0.3
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	8	0.3
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	10	0.3
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	10	0.3
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	10	0.3
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD21	9	0.3
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD22	9	0.3
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD23	9	0.3
(1,87)	1:101:A:LYS:HD2	1:104:A:GLU:HG2	6	0.3
(1,87)	1:101:A:LYS:HD2	1:104:A:GLU:HG3	6	0.3
(1,87)	1:101:A:LYS:HD3	1:104:A:GLU:HG2	6	0.3
(1,87)	1:101:A:LYS:HD3	1:104:A:GLU:HG3	6	0.3
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	1	0.3
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	1	0.3
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG11	8	0.29
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG12	8	0.29
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG13	8	0.29
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG21	8	0.29
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG22	8	0.29
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG23	8	0.29
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG11	8	0.29
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG12	8	0.29
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG13	8	0.29
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG21	8	0.29
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG22	8	0.29
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG23	8	0.29
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB2	3	0.29
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB3	3	0.29
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB2	3	0.29
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB3	3	0.29
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	7	0.29
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	7	0.29
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	7	0.29
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	7	0.29
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	7	0.29
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	1	0.29
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	1	0.29
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	3	0.29
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	3	0.29
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	3	0.29
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	3	0.29
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	3	0.29
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	3	0.29
(1,1419)	1:82:A:VAL:HG11	1:170:A:GLN:HG2	3	0.29
(1,1419)	1:82:A:VAL:HG11	1:170:A:GLN:HG3	3	0.29
(1,1419)	1:82:A:VAL:HG12	1:170:A:GLN:HG2	3	0.29
(1,1419)	1:82:A:VAL:HG12	1:170:A:GLN:HG3	3	0.29
(1,1419)	1:82:A:VAL:HG13	1:170:A:GLN:HG2	3	0.29
(1,1419)	1:82:A:VAL:HG13	1:170:A:GLN:HG3	3	0.29
(1,1419)	1:82:A:VAL:HG21	1:170:A:GLN:HG2	3	0.29
(1,1419)	1:82:A:VAL:HG21	1:170:A:GLN:HG3	3	0.29
(1,1419)	1:82:A:VAL:HG22	1:170:A:GLN:HG2	3	0.29
(1,1419)	1:82:A:VAL:HG22	1:170:A:GLN:HG3	3	0.29
(1,1419)	1:82:A:VAL:HG23	1:170:A:GLN:HG2	3	0.29
(1,1419)	1:82:A:VAL:HG23	1:170:A:GLN:HG3	3	0.29
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG11	8	0.29
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG12	8	0.29
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG13	8	0.29
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG21	8	0.29
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG22	8	0.29
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG23	8	0.29
(1,1386)	1:64:A:LEU:HD11	1:69:A:LYS:H	7	0.29
(1,1386)	1:64:A:LEU:HD12	1:69:A:LYS:H	7	0.29
(1,1386)	1:64:A:LEU:HD13	1:69:A:LYS:H	7	0.29
(1,1386)	1:64:A:LEU:HD21	1:69:A:LYS:H	7	0.29
(1,1386)	1:64:A:LEU:HD22	1:69:A:LYS:H	7	0.29
(1,1386)	1:64:A:LEU:HD23	1:69:A:LYS:H	7	0.29
(1,1321)	1:41:A:LYS:HE2	1:121:A:VAL:HG11	4	0.29
(1,1321)	1:41:A:LYS:HE2	1:121:A:VAL:HG12	4	0.29
(1,1321)	1:41:A:LYS:HE2	1:121:A:VAL:HG13	4	0.29
(1,1321)	1:41:A:LYS:HE2	1:121:A:VAL:HG21	4	0.29
(1,1321)	1:41:A:LYS:HE2	1:121:A:VAL:HG22	4	0.29
(1,1321)	1:41:A:LYS:HE2	1:121:A:VAL:HG23	4	0.29
(1,1321)	1:41:A:LYS:HE3	1:121:A:VAL:HG11	4	0.29
(1,1321)	1:41:A:LYS:HE3	1:121:A:VAL:HG12	4	0.29
(1,1321)	1:41:A:LYS:HE3	1:121:A:VAL:HG13	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1321)	1:41:A:LYS:HE3	1:121:A:VAL:HG21	4	0.29
(1,1321)	1:41:A:LYS:HE3	1:121:A:VAL:HG22	4	0.29
(1,1321)	1:41:A:LYS:HE3	1:121:A:VAL:HG23	4	0.29
(1,1224)	1:82:A:VAL:HG11	1:170:A:GLN:H	2	0.29
(1,1224)	1:82:A:VAL:HG12	1:170:A:GLN:H	2	0.29
(1,1224)	1:82:A:VAL:HG13	1:170:A:GLN:H	2	0.29
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	6	0.29
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	6	0.29
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	6	0.29
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB1	5	0.29
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB2	5	0.29
(1,799)	1:111:A:PHE:HD1	1:149:A:ALA:HB3	5	0.29
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB1	5	0.29
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB2	5	0.29
(1,799)	1:111:A:PHE:HD2	1:149:A:ALA:HB3	5	0.29
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	1	0.29
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	1	0.29
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	1	0.29
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	1	0.29
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	1	0.29
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	1	0.29
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD11	1	0.29
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD12	1	0.29
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD13	1	0.29
(1,669)	1:113:A:ALA:HA	1:116:A:ASP:HB3	4	0.29
(1,618)	1:146:A:ILE:HG21	1:152:A:LEU:HA	6	0.29
(1,618)	1:146:A:ILE:HG22	1:152:A:LEU:HA	6	0.29
(1,618)	1:146:A:ILE:HG23	1:152:A:LEU:HA	6	0.29
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD11	6	0.29
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD12	6	0.29
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD13	6	0.29
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	5	0.29
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	5	0.29
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	5	0.29
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG2	2	0.29
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG3	2	0.29
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG2	1	0.29
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG3	1	0.29
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG2	1	0.29
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG3	1	0.29
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG2	1	0.29
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG3	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD21	1	0.29
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD22	1	0.29
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD23	1	0.29
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD21	3	0.29
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD22	3	0.29
(1,229)	1:33:A:LEU:H	1:33:A:LEU:HD23	3	0.29
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG2	3	0.29
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG3	3	0.29
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	6	0.29
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	9	0.29
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	9	0.29
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	9	0.29
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	9	0.29
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	9	0.29
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	9	0.29
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG2	9	0.29
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG3	9	0.29
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG2	9	0.29
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG3	9	0.29
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD11	7	0.28
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD12	7	0.28
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD13	7	0.28
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD21	7	0.28
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD22	7	0.28
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD23	7	0.28
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB2	10	0.28
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB3	10	0.28
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB2	10	0.28
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB3	10	0.28
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD11	3	0.28
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD12	3	0.28
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD13	3	0.28
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD21	3	0.28
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD22	3	0.28
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD23	3	0.28
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD11	3	0.28
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD12	3	0.28
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD13	3	0.28
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD21	3	0.28
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD22	3	0.28
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD23	3	0.28
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	6	0.28
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	6	0.28
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	6	0.28
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	6	0.28
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	6	0.28
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	6	0.28
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	6	0.28
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	6	0.28
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	6	0.28
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	6	0.28
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	6	0.28
(1,1244)	1:26:A:VAL:HG11	1:30:A:ASN:HD21	8	0.28
(1,1244)	1:26:A:VAL:HG11	1:30:A:ASN:HD22	8	0.28
(1,1244)	1:26:A:VAL:HG12	1:30:A:ASN:HD21	8	0.28
(1,1244)	1:26:A:VAL:HG12	1:30:A:ASN:HD22	8	0.28
(1,1244)	1:26:A:VAL:HG13	1:30:A:ASN:HD21	8	0.28
(1,1244)	1:26:A:VAL:HG13	1:30:A:ASN:HD22	8	0.28
(1,1244)	1:26:A:VAL:HG21	1:30:A:ASN:HD21	8	0.28
(1,1244)	1:26:A:VAL:HG21	1:30:A:ASN:HD22	8	0.28
(1,1244)	1:26:A:VAL:HG22	1:30:A:ASN:HD21	8	0.28
(1,1244)	1:26:A:VAL:HG22	1:30:A:ASN:HD22	8	0.28
(1,1244)	1:26:A:VAL:HG23	1:30:A:ASN:HD21	8	0.28
(1,1244)	1:26:A:VAL:HG23	1:30:A:ASN:HD22	8	0.28
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	8	0.28
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	8	0.28
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	8	0.28
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	10	0.28
(1,703)	1:92:A:LEU:HA	1:95:A:ILE:HG12	8	0.28
(1,703)	1:92:A:LEU:HA	1:95:A:ILE:HG13	8	0.28
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA2	8	0.28
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA3	8	0.28
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA2	8	0.28
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA3	8	0.28
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA2	8	0.28
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA3	8	0.28
(1,478)	1:99:A:ALA:HB1	1:153:A:LEU:HG	10	0.28
(1,478)	1:99:A:ALA:HB2	1:153:A:LEU:HG	10	0.28
(1,478)	1:99:A:ALA:HB3	1:153:A:LEU:HG	10	0.28
(1,456)	1:152:A:LEU:HA	1:154:A:ALA:HB1	6	0.28
(1,456)	1:152:A:LEU:HA	1:154:A:ALA:HB2	6	0.28
(1,456)	1:152:A:LEU:HA	1:154:A:ALA:HB3	6	0.28
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	5	0.28
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	5	0.28
(1,318)	1:102:A:LEU:HD11	1:106:A:GLY:H	7	0.28
(1,318)	1:102:A:LEU:HD12	1:106:A:GLY:H	7	0.28
(1,318)	1:102:A:LEU:HD13	1:106:A:GLY:H	7	0.28
(1,52)	1:160:A:GLU:H	1:160:A:GLU:HG3	7	0.28
(1,1629)	1:143:A:ASN:HA	1:143:A:ASN:HD21	8	0.27
(1,1629)	1:143:A:ASN:HA	1:143:A:ASN:HD22	8	0.27
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	3	0.27
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	3	0.27
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	3	0.27
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	3	0.27
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	3	0.27
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	3	0.27
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	4	0.27
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	4	0.27
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	4	0.27
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	4	0.27
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	4	0.27
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	4	0.27
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	6	0.27
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	6	0.27
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB2	6	0.27
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB3	6	0.27
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG11	5	0.27
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG12	5	0.27
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG13	5	0.27
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG21	5	0.27
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG22	5	0.27
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG23	5	0.27
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG2	5	0.27
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG3	5	0.27
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG2	5	0.27
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG3	5	0.27
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG2	5	0.27
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG3	5	0.27
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG2	5	0.27
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG3	5	0.27
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG2	5	0.27
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG3	5	0.27
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG2	5	0.27
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG3	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:89:A:GLY:H	1:90:A:LYS:HG2	9	0.27
(1,1232)	1:89:A:GLY:H	1:90:A:LYS:HG3	9	0.27
(1,1209)	1:64:A:LEU:HD21	1:67:A:GLY:H	6	0.27
(1,1209)	1:64:A:LEU:HD22	1:67:A:GLY:H	6	0.27
(1,1209)	1:64:A:LEU:HD23	1:67:A:GLY:H	6	0.27
(1,954)	1:26:A:VAL:H	1:26:A:VAL:HB	5	0.27
(1,748)	1:39:A:ASP:HA	1:42:A:ASN:HD22	10	0.27
(1,661)	1:157:A:ALA:HA	1:159:A:ILE:H	5	0.27
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	10	0.27
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	10	0.27
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	10	0.27
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA2	4	0.27
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA3	4	0.27
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA2	4	0.27
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA3	4	0.27
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA2	4	0.27
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA3	4	0.27
(1,512)	1:114:A:MET:H	1:114:A:MET:HE1	10	0.27
(1,512)	1:114:A:MET:H	1:114:A:MET:HE2	10	0.27
(1,512)	1:114:A:MET:H	1:114:A:MET:HE3	10	0.27
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	3	0.27
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	3	0.27
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	3	0.27
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG2	6	0.27
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG3	6	0.27
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	1	0.27
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG2	6	0.27
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG3	6	0.27
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG2	6	0.27
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG3	6	0.27
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	6	0.27
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	6	0.27
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	1	0.26
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	1	0.26
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	1	0.26
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	1	0.26
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	1	0.26
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	1	0.26
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	1	0.26
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	1	0.26
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	1	0.26
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	1	0.26
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	1	0.26
(1,1232)	1:89:A:GLY:H	1:90:A:LYS:HG2	7	0.26
(1,1232)	1:89:A:GLY:H	1:90:A:LYS:HG3	7	0.26
(1,1219)	1:146:A:ILE:HD11	1:149:A:ALA:H	8	0.26
(1,1219)	1:146:A:ILE:HD12	1:149:A:ALA:H	8	0.26
(1,1219)	1:146:A:ILE:HD13	1:149:A:ALA:H	8	0.26
(1,1184)	1:168:A:GLU:H	1:169:A:LYS:HD2	2	0.26
(1,1184)	1:168:A:GLU:H	1:169:A:LYS:HD3	2	0.26
(1,1151)	1:141:A:SER:H	1:146:A:ILE:HB	8	0.26
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	6	0.26
(1,781)	1:85:A:ILE:HG21	1:88:A:THR:HA	9	0.26
(1,781)	1:85:A:ILE:HG22	1:88:A:THR:HA	9	0.26
(1,781)	1:85:A:ILE:HG23	1:88:A:THR:HA	9	0.26
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	7	0.26
(1,652)	1:25:A:LEU:HA	1:25:A:LEU:HG	10	0.26
(1,618)	1:146:A:ILE:HG21	1:152:A:LEU:HA	9	0.26
(1,618)	1:146:A:ILE:HG22	1:152:A:LEU:HA	9	0.26
(1,618)	1:146:A:ILE:HG23	1:152:A:LEU:HA	9	0.26
(1,499)	1:114:A:MET:HE1	1:156:A:LYS:H	9	0.26
(1,499)	1:114:A:MET:HE2	1:156:A:LYS:H	9	0.26
(1,499)	1:114:A:MET:HE3	1:156:A:LYS:H	9	0.26
(1,478)	1:99:A:ALA:HB1	1:153:A:LEU:HG	6	0.26
(1,478)	1:99:A:ALA:HB2	1:153:A:LEU:HG	6	0.26
(1,478)	1:99:A:ALA:HB3	1:153:A:LEU:HG	6	0.26
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	1	0.26
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	1	0.26
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	1	0.26
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	3	0.26
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	3	0.26
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	3	0.26
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	3	0.26
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	3	0.26
(1,346)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	3	0.26
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	3	0.26
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	3	0.26
(1,346)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	3	0.26
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	3	0.26
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	3	0.26
(1,346)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	3	0.26
(1,143)	1:118:A:MET:HG2	1:159:A:ILE:HD11	10	0.26
(1,143)	1:118:A:MET:HG2	1:159:A:ILE:HD12	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:118:A:MET:HG2	1:159:A:ILE:HD13	10	0.26
(1,143)	1:118:A:MET:HG3	1:159:A:ILE:HD11	10	0.26
(1,143)	1:118:A:MET:HG3	1:159:A:ILE:HD12	10	0.26
(1,143)	1:118:A:MET:HG3	1:159:A:ILE:HD13	10	0.26
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG2	7	0.25
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG3	7	0.25
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG2	7	0.25
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG3	7	0.25
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG2	7	0.25
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG3	7	0.25
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG2	6	0.25
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG3	6	0.25
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG2	6	0.25
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG3	6	0.25
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	6	0.25
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	6	0.25
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	6	0.25
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	6	0.25
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	6	0.25
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	6	0.25
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB2	9	0.25
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB3	9	0.25
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	6	0.25
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	6	0.25
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	6	0.25
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	6	0.25
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	6	0.25
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	6	0.25
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD11	8	0.25
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD12	8	0.25
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD13	8	0.25
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD21	8	0.25
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD22	8	0.25
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD23	8	0.25
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD11	2	0.25
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD12	2	0.25
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD13	2	0.25
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD21	2	0.25
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD22	2	0.25
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD23	2	0.25
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD11	2	0.25
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD12	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD13	2	0.25
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD21	2	0.25
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD22	2	0.25
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD23	2	0.25
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD11	2	0.25
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD12	2	0.25
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD13	2	0.25
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD21	2	0.25
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD22	2	0.25
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD23	2	0.25
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	8	0.25
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	8	0.25
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	8	0.25
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD2	9	0.25
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD3	9	0.25
(1,652)	1:25:A:LEU:HA	1:25:A:LEU:HG	4	0.25
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	9	0.25
(1,458)	1:85:A:ILE:HG21	1:164:A:LYS:HA	3	0.25
(1,458)	1:85:A:ILE:HG22	1:164:A:LYS:HA	3	0.25
(1,458)	1:85:A:ILE:HG23	1:164:A:LYS:HA	3	0.25
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	6	0.25
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	6	0.25
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	6	0.25
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD21	2	0.25
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD22	2	0.25
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD23	2	0.25
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD21	6	0.25
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD22	6	0.25
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD23	6	0.25
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB2	1	0.25
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB3	1	0.25
(1,18)	1:25:A:LEU:HB2	1:26:A:VAL:HA	4	0.25
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	9	0.24
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	9	0.24
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	9	0.24
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	9	0.24
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	9	0.24
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	9	0.24
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD11	5	0.24
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD12	5	0.24
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD13	5	0.24
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD21	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD22	5	0.24
(1,1462)	1:96:A:GLU:HA	1:153:A:LEU:HD23	5	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD11	7	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD12	7	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD13	7	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD21	7	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD22	7	0.24
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD23	7	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD11	7	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD12	7	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD13	7	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD21	7	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD22	7	0.24
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD23	7	0.24
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	3	0.24
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	3	0.24
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	3	0.24
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	3	0.24
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	3	0.24
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	3	0.24
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	3	0.24
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	3	0.24
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	3	0.24
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	3	0.24
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	3	0.24
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	3	0.24
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	7	0.24
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	7	0.24
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	7	0.24
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	7	0.24
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	7	0.24
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	7	0.24
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD11	9	0.24
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD12	9	0.24
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD13	9	0.24
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD21	9	0.24
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD22	9	0.24
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD23	9	0.24
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD11	9	0.24
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD12	9	0.24
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD13	9	0.24
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD21	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD22	9	0.24
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD23	9	0.24
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG21	9	0.24
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG22	9	0.24
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG23	9	0.24
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG21	9	0.24
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG22	9	0.24
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG23	9	0.24
(1,1195)	1:111:A:PHE:H	1:147:A:ASN:HA	5	0.24
(1,1168)	1:102:A:LEU:HD21	1:106:A:GLY:H	5	0.24
(1,1168)	1:102:A:LEU:HD22	1:106:A:GLY:H	5	0.24
(1,1168)	1:102:A:LEU:HD23	1:106:A:GLY:H	5	0.24
(1,1117)	1:101:A:LYS:HG2	1:104:A:GLU:H	9	0.24
(1,1117)	1:101:A:LYS:HG3	1:104:A:GLU:H	9	0.24
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG2	8	0.24
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG3	8	0.24
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	1	0.24
(1,755)	1:44:A:ILE:HD11	1:124:A:SER:H	10	0.24
(1,755)	1:44:A:ILE:HD12	1:124:A:SER:H	10	0.24
(1,755)	1:44:A:ILE:HD13	1:124:A:SER:H	10	0.24
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	9	0.24
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	9	0.24
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	1	0.24
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	1	0.24
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	1	0.24
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	4	0.24
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	4	0.24
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	4	0.24
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	4	0.24
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	4	0.24
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	4	0.24
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG21	8	0.24
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG22	8	0.24
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG23	8	0.24
(1,313)	1:146:A:ILE:HG21	1:152:A:LEU:HD11	9	0.24
(1,313)	1:146:A:ILE:HG21	1:152:A:LEU:HD12	9	0.24
(1,313)	1:146:A:ILE:HG21	1:152:A:LEU:HD13	9	0.24
(1,313)	1:146:A:ILE:HG22	1:152:A:LEU:HD11	9	0.24
(1,313)	1:146:A:ILE:HG22	1:152:A:LEU:HD12	9	0.24
(1,313)	1:146:A:ILE:HG22	1:152:A:LEU:HD13	9	0.24
(1,313)	1:146:A:ILE:HG23	1:152:A:LEU:HD11	9	0.24
(1,313)	1:146:A:ILE:HG23	1:152:A:LEU:HD12	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:146:A:ILE:HG23	1:152:A:LEU:HD13	9	0.24
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	8	0.24
(1,174)	1:65:A:LYS:HA	1:65:A:LYS:HD2	10	0.24
(1,174)	1:65:A:LYS:HA	1:65:A:LYS:HD3	10	0.24
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD2	3	0.24
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD3	3	0.24
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	4	0.24
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	4	0.24
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG11	2	0.23
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG12	2	0.23
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG13	2	0.23
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG21	2	0.23
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG22	2	0.23
(1,1684)	1:164:A:LYS:HE2	1:165:A:VAL:HG23	2	0.23
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG11	2	0.23
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG12	2	0.23
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG13	2	0.23
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG21	2	0.23
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG22	2	0.23
(1,1684)	1:164:A:LYS:HE3	1:165:A:VAL:HG23	2	0.23
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG21	3	0.23
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG22	3	0.23
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG23	3	0.23
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG21	3	0.23
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG22	3	0.23
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG23	3	0.23
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG21	3	0.23
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG22	3	0.23
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG23	3	0.23
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG21	3	0.23
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG22	3	0.23
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG23	3	0.23
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG21	3	0.23
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG22	3	0.23
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG23	3	0.23
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG21	3	0.23
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG22	3	0.23
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG23	3	0.23
(1,1592)	1:133:A:LEU:HD11	1:165:A:VAL:HB	6	0.23
(1,1592)	1:133:A:LEU:HD12	1:165:A:VAL:HB	6	0.23
(1,1592)	1:133:A:LEU:HD13	1:165:A:VAL:HB	6	0.23
(1,1592)	1:133:A:LEU:HD21	1:165:A:VAL:HB	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:133:A:LEU:HD22	1:165:A:VAL:HB	6	0.23
(1,1592)	1:133:A:LEU:HD23	1:165:A:VAL:HB	6	0.23
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	2	0.23
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	2	0.23
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD11	7	0.23
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD12	7	0.23
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD13	7	0.23
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD11	7	0.23
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD12	7	0.23
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD13	7	0.23
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	1	0.23
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	1	0.23
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	1	0.23
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	1	0.23
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	1	0.23
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	1	0.23
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG2	2	0.23
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG3	2	0.23
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG2	6	0.23
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG3	6	0.23
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG2	7	0.23
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG3	7	0.23
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	6	0.23
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	6	0.23
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	6	0.23
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	6	0.23
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	6	0.23
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	6	0.23
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	5	0.23
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	5	0.23
(1,1493)	1:102:A:LEU:HD11	1:111:A:PHE:HD1	5	0.23
(1,1493)	1:102:A:LEU:HD11	1:111:A:PHE:HD2	5	0.23
(1,1493)	1:102:A:LEU:HD12	1:111:A:PHE:HD1	5	0.23
(1,1493)	1:102:A:LEU:HD12	1:111:A:PHE:HD2	5	0.23
(1,1493)	1:102:A:LEU:HD13	1:111:A:PHE:HD1	5	0.23
(1,1493)	1:102:A:LEU:HD13	1:111:A:PHE:HD2	5	0.23
(1,1493)	1:102:A:LEU:HD21	1:111:A:PHE:HD1	5	0.23
(1,1493)	1:102:A:LEU:HD21	1:111:A:PHE:HD2	5	0.23
(1,1493)	1:102:A:LEU:HD22	1:111:A:PHE:HD1	5	0.23
(1,1493)	1:102:A:LEU:HD22	1:111:A:PHE:HD2	5	0.23
(1,1493)	1:102:A:LEU:HD23	1:111:A:PHE:HD1	5	0.23
(1,1493)	1:102:A:LEU:HD23	1:111:A:PHE:HD2	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD11	9	0.23
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD12	9	0.23
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD13	9	0.23
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD21	9	0.23
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD22	9	0.23
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD23	9	0.23
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD11	9	0.23
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD12	9	0.23
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD13	9	0.23
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD21	9	0.23
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD22	9	0.23
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD23	9	0.23
(1,1418)	1:82:A:VAL:HG11	1:170:A:GLN:H	4	0.23
(1,1418)	1:82:A:VAL:HG12	1:170:A:GLN:H	4	0.23
(1,1418)	1:82:A:VAL:HG13	1:170:A:GLN:H	4	0.23
(1,1418)	1:82:A:VAL:HG21	1:170:A:GLN:H	4	0.23
(1,1418)	1:82:A:VAL:HG22	1:170:A:GLN:H	4	0.23
(1,1418)	1:82:A:VAL:HG23	1:170:A:GLN:H	4	0.23
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG11	1	0.23
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG12	1	0.23
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG13	1	0.23
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG21	1	0.23
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG22	1	0.23
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG23	1	0.23
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG11	1	0.23
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG12	1	0.23
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG13	1	0.23
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG21	1	0.23
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG22	1	0.23
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG23	1	0.23
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD1	7	0.23
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD2	7	0.23
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD1	7	0.23
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD2	7	0.23
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD1	7	0.23
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD2	7	0.23
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD1	7	0.23
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD2	7	0.23
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD1	7	0.23
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD2	7	0.23
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD1	7	0.23
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	4	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	4	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	4	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	4	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	4	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	4	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	4	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	4	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	4	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	4	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	4	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	4	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	8	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	8	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	8	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	8	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	8	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	8	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	8	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	8	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	8	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	8	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	8	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	8	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	9	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	9	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	9	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	9	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	9	0.23
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	9	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	9	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	9	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	9	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	9	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	9	0.23
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	9	0.23
(1,1327)	1:42:A:ASN:HD21	1:45:A:LEU:HB2	9	0.23
(1,1327)	1:42:A:ASN:HD21	1:45:A:LEU:HB3	9	0.23
(1,1327)	1:42:A:ASN:HD22	1:45:A:LEU:HB2	9	0.23
(1,1327)	1:42:A:ASN:HD22	1:45:A:LEU:HB3	9	0.23
(1,1214)	1:60:A:ALA:H	1:61:A:PHE:HD1	10	0.23
(1,1214)	1:60:A:ALA:H	1:61:A:PHE:HD2	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:111:A:PHE:H	1:147:A:ASN:HA	9	0.23
(1,1168)	1:102:A:LEU:HD21	1:106:A:GLY:H	10	0.23
(1,1168)	1:102:A:LEU:HD22	1:106:A:GLY:H	10	0.23
(1,1168)	1:102:A:LEU:HD23	1:106:A:GLY:H	10	0.23
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	10	0.23
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	10	0.23
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	10	0.23
(1,1041)	1:159:A:ILE:HB	1:162:A:GLN:H	5	0.23
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	5	0.23
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	5	0.23
(1,862)	1:114:A:MET:HE1	1:155:A:ALA:H	2	0.23
(1,862)	1:114:A:MET:HE2	1:155:A:ALA:H	2	0.23
(1,862)	1:114:A:MET:HE3	1:155:A:ALA:H	2	0.23
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD11	9	0.23
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD12	9	0.23
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD13	9	0.23
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	2	0.23
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	2	0.23
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD11	4	0.23
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD12	4	0.23
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD13	4	0.23
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD11	7	0.23
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD12	7	0.23
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD13	7	0.23
(1,502)	1:63:A:GLY:H	1:66:A:THR:HA	10	0.23
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	9	0.23
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	9	0.23
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	9	0.23
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	9	0.23
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	9	0.23
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	9	0.23
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	9	0.23
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	9	0.23
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	9	0.23
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	2	0.23
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	2	0.23
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	2	0.23
(1,204)	1:77:A:LEU:HG	1:81:A:LYS:H	1	0.23
(1,188)	1:153:A:LEU:H	1:153:A:LEU:HG	7	0.23
(1,102)	1:158:A:GLN:H	1:158:A:GLN:HG2	7	0.23
(1,93)	1:139:A:GLU:H	1:139:A:GLU:HG2	6	0.23
(1,93)	1:139:A:GLU:H	1:139:A:GLU:HG3	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG2	3	0.23
(1,71)	1:140:A:GLU:H	1:140:A:GLU:HG3	3	0.23
(1,1666)	1:159:A:ILE:HA	1:162:A:GLN:HG2	3	0.22
(1,1666)	1:159:A:ILE:HA	1:162:A:GLN:HG3	3	0.22
(1,1612)	1:137:A:VAL:HB	1:158:A:GLN:HE21	9	0.22
(1,1612)	1:137:A:VAL:HB	1:158:A:GLN:HE22	9	0.22
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB2	2	0.22
(1,1606)	1:136:A:ARG:HG2	1:139:A:GLU:HB3	2	0.22
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB2	2	0.22
(1,1606)	1:136:A:ARG:HG3	1:139:A:GLU:HB3	2	0.22
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	8	0.22
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	8	0.22
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	9	0.22
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	9	0.22
(1,1572)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	9	0.22
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG21	9	0.22
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG22	9	0.22
(1,1572)	1:129:A:GLY:HA3	1:131:A:ILE:HG23	9	0.22
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	8	0.22
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	8	0.22
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	8	0.22
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	8	0.22
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	8	0.22
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	8	0.22
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	8	0.22
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	8	0.22
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	8	0.22
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	8	0.22
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	8	0.22
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	8	0.22
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	8	0.22
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	8	0.22
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	8	0.22
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	8	0.22
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	8	0.22
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	8	0.22
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD11	3	0.22
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD12	3	0.22
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD13	3	0.22
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD21	3	0.22
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD22	3	0.22
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD23	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD11	3	0.22
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD12	3	0.22
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD13	3	0.22
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD21	3	0.22
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD22	3	0.22
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD23	3	0.22
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB2	2	0.22
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB3	2	0.22
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB2	2	0.22
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB3	2	0.22
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB2	2	0.22
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB3	2	0.22
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB2	2	0.22
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB3	2	0.22
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB2	2	0.22
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB3	2	0.22
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB2	2	0.22
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB3	2	0.22
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	7	0.22
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	7	0.22
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	7	0.22
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	7	0.22
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	7	0.22
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	7	0.22
(1,1390)	1:69:A:LYS:HA	1:69:A:LYS:HG2	3	0.22
(1,1390)	1:69:A:LYS:HA	1:69:A:LYS:HG3	3	0.22
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB2	5	0.22
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB3	5	0.22
(1,1344)	1:47:A:ILE:HD11	1:83:A:GLN:HG2	3	0.22
(1,1344)	1:47:A:ILE:HD11	1:83:A:GLN:HG3	3	0.22
(1,1344)	1:47:A:ILE:HD12	1:83:A:GLN:HG2	3	0.22
(1,1344)	1:47:A:ILE:HD12	1:83:A:GLN:HG3	3	0.22
(1,1344)	1:47:A:ILE:HD13	1:83:A:GLN:HG2	3	0.22
(1,1344)	1:47:A:ILE:HD13	1:83:A:GLN:HG3	3	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	4	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	4	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	4	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	4	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	4	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	4	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	10	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	10	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	10	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	10	0.22
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	10	0.22
(1,1220)	1:131:A:ILE:H	1:132:A:GLY:H	4	0.22
(1,1214)	1:60:A:ALA:H	1:61:A:PHE:HD1	9	0.22
(1,1214)	1:60:A:ALA:H	1:61:A:PHE:HD2	9	0.22
(1,1158)	1:137:A:VAL:HG21	1:141:A:SER:H	1	0.22
(1,1158)	1:137:A:VAL:HG22	1:141:A:SER:H	1	0.22
(1,1158)	1:137:A:VAL:HG23	1:141:A:SER:H	1	0.22
(1,1140)	1:35:A:SER:H	1:38:A:LYS:HG2	5	0.22
(1,1140)	1:35:A:SER:H	1:38:A:LYS:HG3	5	0.22
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	2	0.22
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	2	0.22
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	2	0.22
(1,954)	1:26:A:VAL:H	1:26:A:VAL:HB	7	0.22
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG21	4	0.22
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG22	4	0.22
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG23	4	0.22
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG21	4	0.22
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG22	4	0.22
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG23	4	0.22
(1,755)	1:44:A:ILE:HD11	1:124:A:SER:H	6	0.22
(1,755)	1:44:A:ILE:HD12	1:124:A:SER:H	6	0.22
(1,755)	1:44:A:ILE:HD13	1:124:A:SER:H	6	0.22
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	5	0.22
(1,694)	1:114:A:MET:HE1	1:118:A:MET:HB3	1	0.22
(1,694)	1:114:A:MET:HE2	1:118:A:MET:HB3	1	0.22
(1,694)	1:114:A:MET:HE3	1:118:A:MET:HB3	1	0.22
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD11	5	0.22
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD12	5	0.22
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD13	5	0.22
(1,555)	1:85:A:ILE:HD11	1:167:A:LYS:H	10	0.22
(1,555)	1:85:A:ILE:HD12	1:167:A:LYS:H	10	0.22
(1,555)	1:85:A:ILE:HD13	1:167:A:LYS:H	10	0.22
(1,423)	1:131:A:ILE:HG21	1:132:A:GLY:H	4	0.22
(1,423)	1:131:A:ILE:HG22	1:132:A:GLY:H	4	0.22
(1,423)	1:131:A:ILE:HG23	1:132:A:GLY:H	4	0.22
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG21	3	0.22
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG22	3	0.22
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG23	3	0.22
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG2	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG3	1	0.22
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	1	0.22
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	1	0.22
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	1	0.22
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	1	0.22
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG2	7	0.22
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG3	7	0.22
(1,50)	1:144:A:ASN:H	1:144:A:ASN:HB3	3	0.22
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE2	9	0.22
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE3	9	0.22
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE2	9	0.22
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE3	9	0.22
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	2	0.22
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	2	0.22
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	6	0.22
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	6	0.22
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	1	0.21
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	1	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD11	6	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD12	6	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD13	6	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD21	6	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD22	6	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD23	6	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD11	7	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD12	7	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD13	7	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD21	7	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD22	7	0.21
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD23	7	0.21
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD11	5	0.21
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD12	5	0.21
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD13	5	0.21
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD21	5	0.21
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD22	5	0.21
(1,1450)	1:91:A:PHE:HD1	1:117:A:LEU:HD23	5	0.21
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD11	5	0.21
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD12	5	0.21
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD13	5	0.21
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD21	5	0.21
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD22	5	0.21
(1,1450)	1:91:A:PHE:HD2	1:117:A:LEU:HD23	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	4	0.21
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	4	0.21
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	4	0.21
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	4	0.21
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	4	0.21
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	4	0.21
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	4	0.21
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	4	0.21
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	4	0.21
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	4	0.21
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	4	0.21
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	4	0.21
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG2	10	0.21
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG3	10	0.21
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG2	10	0.21
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG3	10	0.21
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG2	10	0.21
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG3	10	0.21
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG2	10	0.21
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG3	10	0.21
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG2	10	0.21
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG3	10	0.21
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG2	10	0.21
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG3	10	0.21
(1,1349)	1:52:A:THR:HG21	1:56:A:VAL:HG11	2	0.21
(1,1349)	1:52:A:THR:HG21	1:56:A:VAL:HG12	2	0.21
(1,1349)	1:52:A:THR:HG21	1:56:A:VAL:HG13	2	0.21
(1,1349)	1:52:A:THR:HG21	1:56:A:VAL:HG21	2	0.21
(1,1349)	1:52:A:THR:HG21	1:56:A:VAL:HG22	2	0.21
(1,1349)	1:52:A:THR:HG21	1:56:A:VAL:HG23	2	0.21
(1,1349)	1:52:A:THR:HG22	1:56:A:VAL:HG11	2	0.21
(1,1349)	1:52:A:THR:HG22	1:56:A:VAL:HG12	2	0.21
(1,1349)	1:52:A:THR:HG22	1:56:A:VAL:HG13	2	0.21
(1,1349)	1:52:A:THR:HG22	1:56:A:VAL:HG21	2	0.21
(1,1349)	1:52:A:THR:HG22	1:56:A:VAL:HG22	2	0.21
(1,1349)	1:52:A:THR:HG22	1:56:A:VAL:HG23	2	0.21
(1,1349)	1:52:A:THR:HG23	1:56:A:VAL:HG11	2	0.21
(1,1349)	1:52:A:THR:HG23	1:56:A:VAL:HG12	2	0.21
(1,1349)	1:52:A:THR:HG23	1:56:A:VAL:HG13	2	0.21
(1,1349)	1:52:A:THR:HG23	1:56:A:VAL:HG21	2	0.21
(1,1349)	1:52:A:THR:HG23	1:56:A:VAL:HG22	2	0.21
(1,1349)	1:52:A:THR:HG23	1:56:A:VAL:HG23	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	5	0.21
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	5	0.21
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	5	0.21
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	5	0.21
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	5	0.21
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	5	0.21
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB2	6	0.21
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB3	6	0.21
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB2	6	0.21
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB3	6	0.21
(1,1219)	1:146:A:ILE:HD11	1:149:A:ALA:H	2	0.21
(1,1219)	1:146:A:ILE:HD12	1:149:A:ALA:H	2	0.21
(1,1219)	1:146:A:ILE:HD13	1:149:A:ALA:H	2	0.21
(1,1195)	1:111:A:PHE:H	1:147:A:ASN:HA	7	0.21
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	3	0.21
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	4	0.21
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD11	3	0.21
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD12	3	0.21
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD13	3	0.21
(1,811)	1:26:A:VAL:H	1:27:A:GLU:H	5	0.21
(1,748)	1:39:A:ASP:HA	1:42:A:ASN:HD22	8	0.21
(1,740)	1:131:A:ILE:HB	1:132:A:GLY:HA2	4	0.21
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD2	3	0.21
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD3	3	0.21
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	5	0.21
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	5	0.21
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	5	0.21
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD11	3	0.21
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD12	3	0.21
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD13	3	0.21
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD11	3	0.21
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD12	3	0.21
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD13	3	0.21
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	1	0.21
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	1	0.21
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	1	0.21
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	1	0.21
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	1	0.21
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	1	0.21
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	1	0.21
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	1	0.21
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	8	0.21
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	8	0.21
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	8	0.21
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	8	0.21
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	8	0.21
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	8	0.21
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	8	0.21
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	8	0.21
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	8	0.21
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	1	0.21
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	1	0.21
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	1	0.21
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	7	0.21
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	7	0.21
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	7	0.21
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	9	0.21
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	9	0.21
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	9	0.21
(1,340)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	2	0.21
(1,340)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	2	0.21
(1,340)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	2	0.21
(1,340)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	2	0.21
(1,340)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	2	0.21
(1,340)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	2	0.21
(1,283)	1:29:A:THR:HB	1:30:A:ASN:H	5	0.21
(1,209)	1:45:A:LEU:H	1:45:A:LEU:HG	4	0.21
(1,188)	1:153:A:LEU:H	1:153:A:LEU:HG	6	0.21
(1,188)	1:153:A:LEU:H	1:153:A:LEU:HG	10	0.21
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	1	0.21
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	1	0.21
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	1	0.21
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	1	0.21
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	1	0.21
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	1	0.21
(1,82)	1:101:A:LYS:HE2	1:104:A:GLU:HG2	7	0.21
(1,82)	1:101:A:LYS:HE2	1:104:A:GLU:HG3	7	0.21
(1,82)	1:101:A:LYS:HE3	1:104:A:GLU:HG2	7	0.21
(1,82)	1:101:A:LYS:HE3	1:104:A:GLU:HG3	7	0.21
(1,41)	1:37:A:SER:HA	1:39:A:ASP:HB2	2	0.21
(1,18)	1:25:A:LEU:HB2	1:26:A:VAL:HA	7	0.21
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	7	0.21
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:158:A:GLN:HG2	1:161:A:ASN:H	10	0.2
(1,1665)	1:158:A:GLN:HG3	1:161:A:ASN:H	10	0.2
(1,1592)	1:133:A:LEU:HD11	1:165:A:VAL:HB	9	0.2
(1,1592)	1:133:A:LEU:HD12	1:165:A:VAL:HB	9	0.2
(1,1592)	1:133:A:LEU:HD13	1:165:A:VAL:HB	9	0.2
(1,1592)	1:133:A:LEU:HD21	1:165:A:VAL:HB	9	0.2
(1,1592)	1:133:A:LEU:HD22	1:165:A:VAL:HB	9	0.2
(1,1592)	1:133:A:LEU:HD23	1:165:A:VAL:HB	9	0.2
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	7	0.2
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	7	0.2
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	7	0.2
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	7	0.2
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	7	0.2
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	7	0.2
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG2	9	0.2
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG3	9	0.2
(1,1517)	1:112:A:LEU:HD11	1:147:A:ASN:HA	3	0.2
(1,1517)	1:112:A:LEU:HD12	1:147:A:ASN:HA	3	0.2
(1,1517)	1:112:A:LEU:HD13	1:147:A:ASN:HA	3	0.2
(1,1517)	1:112:A:LEU:HD21	1:147:A:ASN:HA	3	0.2
(1,1517)	1:112:A:LEU:HD22	1:147:A:ASN:HA	3	0.2
(1,1517)	1:112:A:LEU:HD23	1:147:A:ASN:HA	3	0.2
(1,1497)	1:106:A:GLY:H	1:110:A:GLN:HB2	10	0.2
(1,1497)	1:106:A:GLY:H	1:110:A:GLN:HB3	10	0.2
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB2	5	0.2
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB3	5	0.2
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	1	0.2
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	1	0.2
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	1	0.2
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	1	0.2
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	1	0.2
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	1	0.2
(1,1426)	1:83:A:GLN:HE21	1:87:A:GLU:HG2	6	0.2
(1,1426)	1:83:A:GLN:HE21	1:87:A:GLU:HG3	6	0.2
(1,1426)	1:83:A:GLN:HE22	1:87:A:GLU:HG2	6	0.2
(1,1426)	1:83:A:GLN:HE22	1:87:A:GLU:HG3	6	0.2
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG2	8	0.2
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG3	8	0.2
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG2	8	0.2
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG3	8	0.2
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG2	8	0.2
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG3	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG2	8	0.2
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG3	8	0.2
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG2	8	0.2
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG3	8	0.2
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG2	8	0.2
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG3	8	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	8	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	8	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	8	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	8	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	8	0.2
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	8	0.2
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD11	1	0.2
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD12	1	0.2
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD13	1	0.2
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD21	1	0.2
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD22	1	0.2
(1,1325)	1:42:A:ASN:HA	1:45:A:LEU:HD23	1	0.2
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB2	3	0.2
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB3	3	0.2
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB2	3	0.2
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB3	3	0.2
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB2	3	0.2
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB3	3	0.2
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB2	3	0.2
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB3	3	0.2
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB2	3	0.2
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB3	3	0.2
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB2	3	0.2
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB3	3	0.2
(1,1285)	1:37:A:SER:HB2	1:121:A:VAL:HG11	8	0.2
(1,1285)	1:37:A:SER:HB2	1:121:A:VAL:HG12	8	0.2
(1,1285)	1:37:A:SER:HB2	1:121:A:VAL:HG13	8	0.2
(1,1285)	1:37:A:SER:HB2	1:121:A:VAL:HG21	8	0.2
(1,1285)	1:37:A:SER:HB2	1:121:A:VAL:HG22	8	0.2
(1,1285)	1:37:A:SER:HB2	1:121:A:VAL:HG23	8	0.2
(1,1285)	1:37:A:SER:HB3	1:121:A:VAL:HG11	8	0.2
(1,1285)	1:37:A:SER:HB3	1:121:A:VAL:HG12	8	0.2
(1,1285)	1:37:A:SER:HB3	1:121:A:VAL:HG13	8	0.2
(1,1285)	1:37:A:SER:HB3	1:121:A:VAL:HG21	8	0.2
(1,1285)	1:37:A:SER:HB3	1:121:A:VAL:HG22	8	0.2
(1,1285)	1:37:A:SER:HB3	1:121:A:VAL:HG23	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1250)	1:30:A:ASN:HD21	1:33:A:LEU:HB2	5	0.2
(1,1250)	1:30:A:ASN:HD21	1:33:A:LEU:HB3	5	0.2
(1,1250)	1:30:A:ASN:HD22	1:33:A:LEU:HB2	5	0.2
(1,1250)	1:30:A:ASN:HD22	1:33:A:LEU:HB3	5	0.2
(1,1243)	1:26:A:VAL:HG11	1:30:A:ASN:HB2	9	0.2
(1,1243)	1:26:A:VAL:HG11	1:30:A:ASN:HB3	9	0.2
(1,1243)	1:26:A:VAL:HG12	1:30:A:ASN:HB2	9	0.2
(1,1243)	1:26:A:VAL:HG12	1:30:A:ASN:HB3	9	0.2
(1,1243)	1:26:A:VAL:HG13	1:30:A:ASN:HB2	9	0.2
(1,1243)	1:26:A:VAL:HG13	1:30:A:ASN:HB3	9	0.2
(1,1243)	1:26:A:VAL:HG21	1:30:A:ASN:HB2	9	0.2
(1,1243)	1:26:A:VAL:HG21	1:30:A:ASN:HB3	9	0.2
(1,1243)	1:26:A:VAL:HG22	1:30:A:ASN:HB2	9	0.2
(1,1243)	1:26:A:VAL:HG22	1:30:A:ASN:HB3	9	0.2
(1,1243)	1:26:A:VAL:HG23	1:30:A:ASN:HB2	9	0.2
(1,1243)	1:26:A:VAL:HG23	1:30:A:ASN:HB3	9	0.2
(1,1182)	1:55:A:GLY:H	1:56:A:VAL:HB	8	0.2
(1,1127)	1:171:A:ASN:H	1:172:A:ILE:HB	2	0.2
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG21	9	0.2
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG22	9	0.2
(1,1089)	1:93:A:LYS:H	1:94:A:ILE:HG23	9	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	6	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	6	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	6	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	9	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	9	0.2
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	9	0.2
(1,1040)	1:162:A:GLN:H	1:165:A:VAL:HB	10	0.2
(1,794)	1:52:A:THR:HG21	1:58:A:PHE:HD1	5	0.2
(1,794)	1:52:A:THR:HG21	1:58:A:PHE:HD2	5	0.2
(1,794)	1:52:A:THR:HG22	1:58:A:PHE:HD1	5	0.2
(1,794)	1:52:A:THR:HG22	1:58:A:PHE:HD2	5	0.2
(1,794)	1:52:A:THR:HG23	1:58:A:PHE:HD1	5	0.2
(1,794)	1:52:A:THR:HG23	1:58:A:PHE:HD2	5	0.2
(1,781)	1:85:A:ILE:HG21	1:88:A:THR:HA	4	0.2
(1,781)	1:85:A:ILE:HG22	1:88:A:THR:HA	4	0.2
(1,781)	1:85:A:ILE:HG23	1:88:A:THR:HA	4	0.2
(1,771)	1:35:A:SER:HB2	1:38:A:LYS:HG2	4	0.2
(1,771)	1:35:A:SER:HB2	1:38:A:LYS:HG3	4	0.2
(1,771)	1:35:A:SER:HB3	1:38:A:LYS:HG2	4	0.2
(1,771)	1:35:A:SER:HB3	1:38:A:LYS:HG3	4	0.2
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD2	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD3	2	0.2
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	10	0.2
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	10	0.2
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	8	0.2
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	8	0.2
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	8	0.2
(1,621)	1:44:A:ILE:HD11	1:47:A:ILE:H	7	0.2
(1,621)	1:44:A:ILE:HD12	1:47:A:ILE:H	7	0.2
(1,621)	1:44:A:ILE:HD13	1:47:A:ILE:H	7	0.2
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD2	9	0.2
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD3	9	0.2
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	10	0.2
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	10	0.2
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	10	0.2
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE1	3	0.2
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE2	3	0.2
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE3	3	0.2
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE1	3	0.2
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE2	3	0.2
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE3	3	0.2
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE1	3	0.2
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE2	3	0.2
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE3	3	0.2
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	5	0.2
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	5	0.2
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	5	0.2
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	5	0.2
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	5	0.2
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	5	0.2
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	5	0.2
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	5	0.2
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	5	0.2
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB1	4	0.2
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB2	4	0.2
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB3	4	0.2
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	2	0.2
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	2	0.2
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	2	0.2
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	7	0.2
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	7	0.2
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	7	0.2
(1,318)	1:102:A:LEU:HD11	1:106:A:GLY:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:102:A:LEU:HD12	1:106:A:GLY:H	3	0.2
(1,318)	1:102:A:LEU:HD13	1:106:A:GLY:H	3	0.2
(1,283)	1:29:A:THR:HB	1:30:A:ASN:H	9	0.2
(1,176)	1:45:A:LEU:HA	1:48:A:LYS:HD2	4	0.2
(1,176)	1:45:A:LEU:HA	1:48:A:LYS:HD3	4	0.2
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	8	0.2
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	8	0.2
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	8	0.2
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	8	0.2
(1,94)	1:139:A:GLU:HG2	1:140:A:GLU:H	1	0.2
(1,94)	1:139:A:GLU:HG3	1:140:A:GLU:H	1	0.2
(1,41)	1:37:A:SER:HA	1:39:A:ASP:HB2	4	0.2
(1,1665)	1:158:A:GLN:HG2	1:161:A:ASN:H	9	0.19
(1,1665)	1:158:A:GLN:HG3	1:161:A:ASN:H	9	0.19
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG2	5	0.19
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG3	5	0.19
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG2	5	0.19
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG3	5	0.19
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG2	5	0.19
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG3	5	0.19
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG2	9	0.19
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG3	9	0.19
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG2	9	0.19
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG3	9	0.19
(1,1612)	1:137:A:VAL:HB	1:158:A:GLN:HE21	10	0.19
(1,1612)	1:137:A:VAL:HB	1:158:A:GLN:HE22	10	0.19
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG2	3	0.19
(1,1544)	1:119:A:LEU:HA	1:134:A:LYS:HG3	3	0.19
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	8	0.19
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	8	0.19
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	8	0.19
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	8	0.19
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	8	0.19
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	8	0.19
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	8	0.19
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	8	0.19
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	8	0.19
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	8	0.19
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	8	0.19
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	8	0.19
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG11	1	0.19
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG12	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG13	1	0.19
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG21	1	0.19
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG22	1	0.19
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG23	1	0.19
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG11	1	0.19
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG12	1	0.19
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG13	1	0.19
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG21	1	0.19
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG22	1	0.19
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG23	1	0.19
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	1	0.19
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	1	0.19
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	1	0.19
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	1	0.19
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	1	0.19
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	1	0.19
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB2	1	0.19
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB3	1	0.19
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB2	1	0.19
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB3	1	0.19
(1,1228)	1:86:A:VAL:H	1:167:A:LYS:HB2	5	0.19
(1,1228)	1:86:A:VAL:H	1:167:A:LYS:HB3	5	0.19
(1,1040)	1:162:A:GLN:H	1:165:A:VAL:HB	8	0.19
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD11	2	0.19
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD12	2	0.19
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD13	2	0.19
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD11	2	0.19
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD12	2	0.19
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD13	2	0.19
(1,798)	1:61:A:PHE:HA	1:61:A:PHE:HD1	3	0.19
(1,798)	1:61:A:PHE:HA	1:61:A:PHE:HD2	3	0.19
(1,798)	1:61:A:PHE:HA	1:61:A:PHE:HD1	5	0.19
(1,798)	1:61:A:PHE:HA	1:61:A:PHE:HD2	5	0.19
(1,753)	1:88:A:THR:HB	1:91:A:PHE:H	7	0.19
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	5	0.19
(1,716)	1:146:A:ILE:HA	1:151:A:ARG:HD2	3	0.19
(1,716)	1:146:A:ILE:HA	1:151:A:ARG:HD3	3	0.19
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	2	0.19
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	2	0.19
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	4	0.19
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	4	0.19
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	5	0.19
(1,618)	1:146:A:ILE:HG21	1:152:A:LEU:HA	7	0.19
(1,618)	1:146:A:ILE:HG22	1:152:A:LEU:HA	7	0.19
(1,618)	1:146:A:ILE:HG23	1:152:A:LEU:HA	7	0.19
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	3	0.19
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD2	3	0.19
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD3	3	0.19
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	2	0.19
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	2	0.19
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	2	0.19
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	3	0.19
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	3	0.19
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	3	0.19
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	3	0.19
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	3	0.19
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	3	0.19
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	3	0.19
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	3	0.19
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	3	0.19
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	10	0.19
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	10	0.19
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	10	0.19
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	4	0.19
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	4	0.19
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	4	0.19
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD21	4	0.19
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD22	4	0.19
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD23	4	0.19
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	8	0.19
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	8	0.19
(1,218)	1:109:A:GLY:HA2	1:112:A:LEU:HG	6	0.19
(1,218)	1:109:A:GLY:HA3	1:112:A:LEU:HG	6	0.19
(1,204)	1:77:A:LEU:HG	1:81:A:LYS:H	3	0.19
(1,144)	1:95:A:ILE:HD11	1:118:A:MET:HG2	8	0.19
(1,144)	1:95:A:ILE:HD11	1:118:A:MET:HG3	8	0.19
(1,144)	1:95:A:ILE:HD12	1:118:A:MET:HG2	8	0.19
(1,144)	1:95:A:ILE:HD12	1:118:A:MET:HG3	8	0.19
(1,144)	1:95:A:ILE:HD13	1:118:A:MET:HG2	8	0.19
(1,144)	1:95:A:ILE:HD13	1:118:A:MET:HG3	8	0.19
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	10	0.19
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	10	0.19
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	10	0.19
(1,75)	1:59:A:GLU:HA	1:59:A:GLU:HG2	5	0.19
(1,75)	1:59:A:GLU:HA	1:59:A:GLU:HG3	5	0.19
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG2	4	0.19
(1,70)	1:120:A:GLU:H	1:120:A:GLU:HG3	4	0.19
(1,56)	1:172:A:ILE:HB	1:173:A:GLU:H	1	0.19
(1,56)	1:172:A:ILE:HB	1:173:A:GLU:H	8	0.19
(1,33)	1:131:A:ILE:HB	1:132:A:GLY:H	2	0.19
(1,1666)	1:159:A:ILE:HA	1:162:A:GLN:HG2	7	0.18
(1,1666)	1:159:A:ILE:HA	1:162:A:GLN:HG3	7	0.18
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE2	8	0.18
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE3	8	0.18
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE2	8	0.18
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE3	8	0.18
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE2	8	0.18
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE3	8	0.18
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE2	8	0.18
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE3	8	0.18
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE2	8	0.18
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE3	8	0.18
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE2	8	0.18
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE3	8	0.18
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	5	0.18
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	5	0.18
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	5	0.18
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	5	0.18
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	5	0.18
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	5	0.18
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	5	0.18
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	5	0.18
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	5	0.18
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	5	0.18
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	5	0.18
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	5	0.18
(1,1399)	1:70:A:VAL:HG11	1:72:A:SER:HB2	7	0.18
(1,1399)	1:70:A:VAL:HG11	1:72:A:SER:HB3	7	0.18
(1,1399)	1:70:A:VAL:HG12	1:72:A:SER:HB2	7	0.18
(1,1399)	1:70:A:VAL:HG12	1:72:A:SER:HB3	7	0.18
(1,1399)	1:70:A:VAL:HG13	1:72:A:SER:HB2	7	0.18
(1,1399)	1:70:A:VAL:HG13	1:72:A:SER:HB3	7	0.18
(1,1399)	1:70:A:VAL:HG21	1:72:A:SER:HB2	7	0.18
(1,1399)	1:70:A:VAL:HG21	1:72:A:SER:HB3	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1399)	1:70:A:VAL:HG22	1:72:A:SER:HB2	7	0.18
(1,1399)	1:70:A:VAL:HG22	1:72:A:SER:HB3	7	0.18
(1,1399)	1:70:A:VAL:HG23	1:72:A:SER:HB2	7	0.18
(1,1399)	1:70:A:VAL:HG23	1:72:A:SER:HB3	7	0.18
(1,1396)	1:70:A:VAL:HG11	1:71:A:THR:H	7	0.18
(1,1396)	1:70:A:VAL:HG12	1:71:A:THR:H	7	0.18
(1,1396)	1:70:A:VAL:HG13	1:71:A:THR:H	7	0.18
(1,1396)	1:70:A:VAL:HG21	1:71:A:THR:H	7	0.18
(1,1396)	1:70:A:VAL:HG22	1:71:A:THR:H	7	0.18
(1,1396)	1:70:A:VAL:HG23	1:71:A:THR:H	7	0.18
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG21	9	0.18
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG22	9	0.18
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG23	9	0.18
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG21	9	0.18
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG22	9	0.18
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG23	9	0.18
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	1	0.18
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	1	0.18
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	1	0.18
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	1	0.18
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	1	0.18
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	1	0.18
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	1	0.18
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	1	0.18
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	1	0.18
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	1	0.18
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	1	0.18
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	1	0.18
(1,1309)	1:40:A:LEU:HD11	1:121:A:VAL:HB	4	0.18
(1,1309)	1:40:A:LEU:HD12	1:121:A:VAL:HB	4	0.18
(1,1309)	1:40:A:LEU:HD13	1:121:A:VAL:HB	4	0.18
(1,1309)	1:40:A:LEU:HD21	1:121:A:VAL:HB	4	0.18
(1,1309)	1:40:A:LEU:HD22	1:121:A:VAL:HB	4	0.18
(1,1309)	1:40:A:LEU:HD23	1:121:A:VAL:HB	4	0.18
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB2	9	0.18
(1,1286)	1:39:A:ASP:HA	1:42:A:ASN:HB3	9	0.18
(1,1280)	1:37:A:SER:HB2	1:41:A:LYS:HD2	8	0.18
(1,1280)	1:37:A:SER:HB2	1:41:A:LYS:HD3	8	0.18
(1,1280)	1:37:A:SER:HB3	1:41:A:LYS:HD2	8	0.18
(1,1280)	1:37:A:SER:HB3	1:41:A:LYS:HD3	8	0.18
(1,1254)	1:32:A:ALA:HB1	1:117:A:LEU:HD11	4	0.18
(1,1254)	1:32:A:ALA:HB1	1:117:A:LEU:HD12	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1254)	1:32:A:ALA:HB1	1:117:A:LEU:HD13	4	0.18
(1,1254)	1:32:A:ALA:HB1	1:117:A:LEU:HD21	4	0.18
(1,1254)	1:32:A:ALA:HB1	1:117:A:LEU:HD22	4	0.18
(1,1254)	1:32:A:ALA:HB1	1:117:A:LEU:HD23	4	0.18
(1,1254)	1:32:A:ALA:HB2	1:117:A:LEU:HD11	4	0.18
(1,1254)	1:32:A:ALA:HB2	1:117:A:LEU:HD12	4	0.18
(1,1254)	1:32:A:ALA:HB2	1:117:A:LEU:HD13	4	0.18
(1,1254)	1:32:A:ALA:HB2	1:117:A:LEU:HD21	4	0.18
(1,1254)	1:32:A:ALA:HB2	1:117:A:LEU:HD22	4	0.18
(1,1254)	1:32:A:ALA:HB2	1:117:A:LEU:HD23	4	0.18
(1,1254)	1:32:A:ALA:HB3	1:117:A:LEU:HD11	4	0.18
(1,1254)	1:32:A:ALA:HB3	1:117:A:LEU:HD12	4	0.18
(1,1254)	1:32:A:ALA:HB3	1:117:A:LEU:HD13	4	0.18
(1,1254)	1:32:A:ALA:HB3	1:117:A:LEU:HD21	4	0.18
(1,1254)	1:32:A:ALA:HB3	1:117:A:LEU:HD22	4	0.18
(1,1254)	1:32:A:ALA:HB3	1:117:A:LEU:HD23	4	0.18
(1,1208)	1:64:A:LEU:HD11	1:67:A:GLY:H	9	0.18
(1,1208)	1:64:A:LEU:HD12	1:67:A:GLY:H	9	0.18
(1,1208)	1:64:A:LEU:HD13	1:67:A:GLY:H	9	0.18
(1,1184)	1:168:A:GLU:H	1:169:A:LYS:HD2	1	0.18
(1,1184)	1:168:A:GLU:H	1:169:A:LYS:HD3	1	0.18
(1,1147)	1:139:A:GLU:HG2	1:141:A:SER:H	1	0.18
(1,1147)	1:139:A:GLU:HG3	1:141:A:SER:H	1	0.18
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG2	1	0.18
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG3	1	0.18
(1,941)	1:156:A:LYS:HG2	1:160:A:GLU:H	4	0.18
(1,941)	1:156:A:LYS:HG3	1:160:A:GLU:H	4	0.18
(1,886)	1:146:A:ILE:HG21	1:149:A:ALA:H	1	0.18
(1,886)	1:146:A:ILE:HG22	1:149:A:ALA:H	1	0.18
(1,886)	1:146:A:ILE:HG23	1:149:A:ALA:H	1	0.18
(1,802)	1:91:A:PHE:HD1	1:94:A:ILE:HD11	9	0.18
(1,802)	1:91:A:PHE:HD1	1:94:A:ILE:HD12	9	0.18
(1,802)	1:91:A:PHE:HD1	1:94:A:ILE:HD13	9	0.18
(1,802)	1:91:A:PHE:HD2	1:94:A:ILE:HD11	9	0.18
(1,802)	1:91:A:PHE:HD2	1:94:A:ILE:HD12	9	0.18
(1,802)	1:91:A:PHE:HD2	1:94:A:ILE:HD13	9	0.18
(1,781)	1:85:A:ILE:HG21	1:88:A:THR:HA	10	0.18
(1,781)	1:85:A:ILE:HG22	1:88:A:THR:HA	10	0.18
(1,781)	1:85:A:ILE:HG23	1:88:A:THR:HA	10	0.18
(1,694)	1:114:A:MET:HE1	1:118:A:MET:HB3	3	0.18
(1,694)	1:114:A:MET:HE2	1:118:A:MET:HB3	3	0.18
(1,694)	1:114:A:MET:HE3	1:118:A:MET:HB3	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:25:A:LEU:HA	1:25:A:LEU:HG	3	0.18
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB1	5	0.18
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB2	5	0.18
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB3	5	0.18
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB1	5	0.18
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB2	5	0.18
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB3	5	0.18
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB1	5	0.18
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB2	5	0.18
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB3	5	0.18
(1,560)	1:126:A:GLU:HA	1:130:A:ILE:HA	7	0.18
(1,528)	1:114:A:MET:HE1	1:118:A:MET:HG2	9	0.18
(1,528)	1:114:A:MET:HE1	1:118:A:MET:HG3	9	0.18
(1,528)	1:114:A:MET:HE2	1:118:A:MET:HG2	9	0.18
(1,528)	1:114:A:MET:HE2	1:118:A:MET:HG3	9	0.18
(1,528)	1:114:A:MET:HE3	1:118:A:MET:HG2	9	0.18
(1,528)	1:114:A:MET:HE3	1:118:A:MET:HG3	9	0.18
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	7	0.18
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	7	0.18
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	7	0.18
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	7	0.18
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	7	0.18
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	7	0.18
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	9	0.18
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	9	0.18
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	9	0.18
(1,426)	1:85:A:ILE:HG21	1:167:A:LYS:H	3	0.18
(1,426)	1:85:A:ILE:HG22	1:167:A:LYS:H	3	0.18
(1,426)	1:85:A:ILE:HG23	1:167:A:LYS:H	3	0.18
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG2	5	0.18
(1,412)	1:137:A:VAL:HA	1:140:A:GLU:HG3	5	0.18
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	3	0.18
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	3	0.18
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	3	0.18
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	10	0.18
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	10	0.18
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	10	0.18
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG21	1	0.18
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG22	1	0.18
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG23	1	0.18
(1,351)	1:148:A:THR:HG21	1:150:A:GLU:H	7	0.18
(1,351)	1:148:A:THR:HG22	1:150:A:GLU:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:148:A:THR:HG23	1:150:A:GLU:H	7	0.18
(1,307)	1:33:A:LEU:HD11	1:98:A:GLU:HB2	9	0.18
(1,307)	1:33:A:LEU:HD11	1:98:A:GLU:HB3	9	0.18
(1,307)	1:33:A:LEU:HD12	1:98:A:GLU:HB2	9	0.18
(1,307)	1:33:A:LEU:HD12	1:98:A:GLU:HB3	9	0.18
(1,307)	1:33:A:LEU:HD13	1:98:A:GLU:HB2	9	0.18
(1,307)	1:33:A:LEU:HD13	1:98:A:GLU:HB3	9	0.18
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD21	8	0.18
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD22	8	0.18
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD23	8	0.18
(1,270)	1:133:A:LEU:HD11	1:165:A:VAL:HB	1	0.18
(1,270)	1:133:A:LEU:HD12	1:165:A:VAL:HB	1	0.18
(1,270)	1:133:A:LEU:HD13	1:165:A:VAL:HB	1	0.18
(1,246)	1:133:A:LEU:H	1:133:A:LEU:HD21	10	0.18
(1,246)	1:133:A:LEU:H	1:133:A:LEU:HD22	10	0.18
(1,246)	1:133:A:LEU:H	1:133:A:LEU:HD23	10	0.18
(1,204)	1:77:A:LEU:HG	1:81:A:LYS:H	8	0.18
(1,169)	1:139:A:GLU:H	1:140:A:GLU:HB2	10	0.18
(1,169)	1:139:A:GLU:H	1:140:A:GLU:HB3	10	0.18
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD2	1	0.18
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD3	1	0.18
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE2	3	0.18
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE3	3	0.18
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE2	3	0.18
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE3	3	0.18
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE2	6	0.18
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE3	6	0.18
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE2	6	0.18
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE3	6	0.18
(1,1697)	1:171:A:ASN:HB2	1:172:A:ILE:HD11	10	0.17
(1,1697)	1:171:A:ASN:HB2	1:172:A:ILE:HD12	10	0.17
(1,1697)	1:171:A:ASN:HB2	1:172:A:ILE:HD13	10	0.17
(1,1697)	1:171:A:ASN:HB3	1:172:A:ILE:HD11	10	0.17
(1,1697)	1:171:A:ASN:HB3	1:172:A:ILE:HD12	10	0.17
(1,1697)	1:171:A:ASN:HB3	1:172:A:ILE:HD13	10	0.17
(1,1674)	1:162:A:GLN:HA	1:162:A:GLN:HE21	7	0.17
(1,1674)	1:162:A:GLN:HA	1:162:A:GLN:HE22	7	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD11	6	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD12	6	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD13	6	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD21	6	0.17
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD22	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD23	6	0.17
(1,1614)	1:137:A:VAL:HG11	1:138:A:LEU:HG	1	0.17
(1,1614)	1:137:A:VAL:HG12	1:138:A:LEU:HG	1	0.17
(1,1614)	1:137:A:VAL:HG13	1:138:A:LEU:HG	1	0.17
(1,1614)	1:137:A:VAL:HG21	1:138:A:LEU:HG	1	0.17
(1,1614)	1:137:A:VAL:HG22	1:138:A:LEU:HG	1	0.17
(1,1614)	1:137:A:VAL:HG23	1:138:A:LEU:HG	1	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	8	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	8	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	8	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	8	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	8	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	8	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	9	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	9	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	9	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	9	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	9	0.17
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	9	0.17
(1,1510)	1:112:A:LEU:HB2	1:115:A:PHE:H	2	0.17
(1,1510)	1:112:A:LEU:HB3	1:115:A:PHE:H	2	0.17
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE2	9	0.17
(1,1478)	1:100:A:LEU:HD11	1:103:A:LYS:HE3	9	0.17
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE2	9	0.17
(1,1478)	1:100:A:LEU:HD12	1:103:A:LYS:HE3	9	0.17
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE2	9	0.17
(1,1478)	1:100:A:LEU:HD13	1:103:A:LYS:HE3	9	0.17
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE2	9	0.17
(1,1478)	1:100:A:LEU:HD21	1:103:A:LYS:HE3	9	0.17
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE2	9	0.17
(1,1478)	1:100:A:LEU:HD22	1:103:A:LYS:HE3	9	0.17
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE2	9	0.17
(1,1478)	1:100:A:LEU:HD23	1:103:A:LYS:HE3	9	0.17
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD11	1	0.17
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD12	1	0.17
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD13	1	0.17
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD21	1	0.17
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD22	1	0.17
(1,1459)	1:95:A:ILE:HB	1:117:A:LEU:HD23	1	0.17
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	9	0.17
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	9	0.17
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	9	0.17
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	9	0.17
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	9	0.17
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	6	0.17
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	6	0.17
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	6	0.17
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	6	0.17
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	6	0.17
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	6	0.17
(1,1260)	1:33:A:LEU:HB2	1:98:A:GLU:HG2	4	0.17
(1,1260)	1:33:A:LEU:HB2	1:98:A:GLU:HG3	4	0.17
(1,1260)	1:33:A:LEU:HB3	1:98:A:GLU:HG2	4	0.17
(1,1260)	1:33:A:LEU:HB3	1:98:A:GLU:HG3	4	0.17
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD11	10	0.17
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD12	10	0.17
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD13	10	0.17
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD21	10	0.17
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD22	10	0.17
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD23	10	0.17
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD11	10	0.17
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD12	10	0.17
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD13	10	0.17
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD21	10	0.17
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD22	10	0.17
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD23	10	0.17
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD11	10	0.17
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD12	10	0.17
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD13	10	0.17
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD21	10	0.17
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD22	10	0.17
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD23	10	0.17
(1,1192)	1:146:A:ILE:H	1:148:A:THR:H	3	0.17
(1,1192)	1:146:A:ILE:H	1:148:A:THR:H	6	0.17
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD11	4	0.17
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD12	4	0.17
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD13	4	0.17
(1,1147)	1:139:A:GLU:HG2	1:141:A:SER:H	5	0.17
(1,1147)	1:139:A:GLU:HG3	1:141:A:SER:H	5	0.17
(1,1083)	1:95:A:ILE:HG21	1:118:A:MET:H	8	0.17
(1,1083)	1:95:A:ILE:HG22	1:118:A:MET:H	8	0.17
(1,1083)	1:95:A:ILE:HG23	1:118:A:MET:H	8	0.17
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	7	0.17
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	7	0.17
(1,1048)	1:37:A:SER:H	1:41:A:LYS:HD2	10	0.17
(1,1048)	1:37:A:SER:H	1:41:A:LYS:HD3	10	0.17
(1,954)	1:26:A:VAL:H	1:26:A:VAL:HB	1	0.17
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD2	3	0.17
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD3	3	0.17
(1,886)	1:146:A:ILE:HG21	1:149:A:ALA:H	6	0.17
(1,886)	1:146:A:ILE:HG22	1:149:A:ALA:H	6	0.17
(1,886)	1:146:A:ILE:HG23	1:149:A:ALA:H	6	0.17
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG21	7	0.17
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG22	7	0.17
(1,797)	1:111:A:PHE:HD1	1:146:A:ILE:HG23	7	0.17
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG21	7	0.17
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG22	7	0.17
(1,797)	1:111:A:PHE:HD2	1:146:A:ILE:HG23	7	0.17
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	8	0.17
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD2	6	0.17
(1,718)	1:134:A:LYS:H	1:134:A:LYS:HD3	6	0.17
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	8	0.17
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	8	0.17
(1,668)	1:113:A:ALA:HA	1:116:A:ASP:HB2	9	0.17
(1,642)	1:38:A:LYS:HB2	1:39:A:ASP:HA	7	0.17
(1,642)	1:38:A:LYS:HB3	1:39:A:ASP:HA	7	0.17
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	6	0.17
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	6	0.17
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	6	0.17
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA2	1	0.17
(1,603)	1:23:A:ILE:HD11	1:24:A:GLY:HA3	1	0.17
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA2	1	0.17
(1,603)	1:23:A:ILE:HD12	1:24:A:GLY:HA3	1	0.17
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA2	1	0.17
(1,603)	1:23:A:ILE:HD13	1:24:A:GLY:HA3	1	0.17
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD11	1	0.17
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD12	1	0.17
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD13	1	0.17
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD11	4	0.17
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD12	4	0.17
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD13	4	0.17
(1,502)	1:63:A:GLY:H	1:66:A:THR:HA	7	0.17
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	6	0.17
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	6	0.17
(1,479)	1:112:A:LEU:HB3	1:113:A:ALA:HB1	9	0.17
(1,479)	1:112:A:LEU:HB3	1:113:A:ALA:HB2	9	0.17
(1,479)	1:112:A:LEU:HB3	1:113:A:ALA:HB3	9	0.17
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	1	0.17
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	1	0.17
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	1	0.17
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	1	0.17
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	1	0.17
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	1	0.17
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	1	0.17
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	1	0.17
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	1	0.17
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	2	0.17
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	2	0.17
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	2	0.17
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	6	0.17
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	6	0.17
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	6	0.17
(1,423)	1:131:A:ILE:HG21	1:132:A:GLY:H	2	0.17
(1,423)	1:131:A:ILE:HG22	1:132:A:GLY:H	2	0.17
(1,423)	1:131:A:ILE:HG23	1:132:A:GLY:H	2	0.17
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD11	10	0.17
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD12	10	0.17
(1,419)	1:44:A:ILE:HA	1:47:A:ILE:HD13	10	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG11	5	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG12	5	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG13	5	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG11	5	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG12	5	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG13	5	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG11	10	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG12	10	0.17
(1,396)	1:48:A:LYS:HB2	1:128:A:VAL:HG13	10	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG11	10	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG12	10	0.17
(1,396)	1:48:A:LYS:HB3	1:128:A:VAL:HG13	10	0.17
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	8	0.17
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	8	0.17
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	8	0.17
(1,351)	1:148:A:THR:HG21	1:150:A:GLU:H	3	0.17
(1,351)	1:148:A:THR:HG22	1:150:A:GLU:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:148:A:THR:HG23	1:150:A:GLU:H	3	0.17
(1,270)	1:133:A:LEU:HD11	1:165:A:VAL:HB	9	0.17
(1,270)	1:133:A:LEU:HD12	1:165:A:VAL:HB	9	0.17
(1,270)	1:133:A:LEU:HD13	1:165:A:VAL:HB	9	0.17
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	6	0.17
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	6	0.17
(1,237)	1:133:A:LEU:HD21	1:162:A:GLN:H	8	0.17
(1,237)	1:133:A:LEU:HD22	1:162:A:GLN:H	8	0.17
(1,237)	1:133:A:LEU:HD23	1:162:A:GLN:H	8	0.17
(1,176)	1:45:A:LEU:HA	1:48:A:LYS:HD2	10	0.17
(1,176)	1:45:A:LEU:HA	1:48:A:LYS:HD3	10	0.17
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB2	7	0.17
(1,162)	1:173:A:GLU:H	1:177:A:GLU:HB3	7	0.17
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	5	0.17
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	5	0.17
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	5	0.17
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	5	0.17
(1,101)	1:83:A:GLN:H	1:83:A:GLN:HG3	8	0.17
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	6	0.17
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	6	0.17
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	6	0.17
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	6	0.17
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	6	0.17
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	6	0.17
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG2	4	0.17
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG3	4	0.17
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG2	4	0.17
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG3	4	0.17
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	10	0.17
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	10	0.17
(1,52)	1:160:A:GLU:H	1:160:A:GLU:HG3	9	0.17
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	1	0.17
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	1	0.17
(1,1585)	1:133:A:LEU:HD11	1:137:A:VAL:HA	5	0.16
(1,1585)	1:133:A:LEU:HD12	1:137:A:VAL:HA	5	0.16
(1,1585)	1:133:A:LEU:HD13	1:137:A:VAL:HA	5	0.16
(1,1585)	1:133:A:LEU:HD21	1:137:A:VAL:HA	5	0.16
(1,1585)	1:133:A:LEU:HD22	1:137:A:VAL:HA	5	0.16
(1,1585)	1:133:A:LEU:HD23	1:137:A:VAL:HA	5	0.16
(1,1556)	1:121:A:VAL:HG11	1:122:A:VAL:H	9	0.16
(1,1556)	1:121:A:VAL:HG12	1:122:A:VAL:H	9	0.16
(1,1556)	1:121:A:VAL:HG13	1:122:A:VAL:H	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:121:A:VAL:HG21	1:122:A:VAL:H	9	0.16
(1,1556)	1:121:A:VAL:HG22	1:122:A:VAL:H	9	0.16
(1,1556)	1:121:A:VAL:HG23	1:122:A:VAL:H	9	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	1	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	1	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	1	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	1	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	1	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	1	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	8	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	8	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	8	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	8	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	8	0.16
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	8	0.16
(1,1517)	1:112:A:LEU:HD11	1:147:A:ASN:HA	6	0.16
(1,1517)	1:112:A:LEU:HD12	1:147:A:ASN:HA	6	0.16
(1,1517)	1:112:A:LEU:HD13	1:147:A:ASN:HA	6	0.16
(1,1517)	1:112:A:LEU:HD21	1:147:A:ASN:HA	6	0.16
(1,1517)	1:112:A:LEU:HD22	1:147:A:ASN:HA	6	0.16
(1,1517)	1:112:A:LEU:HD23	1:147:A:ASN:HA	6	0.16
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	7	0.16
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	7	0.16
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	7	0.16
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	7	0.16
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	7	0.16
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	7	0.16
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	7	0.16
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	7	0.16
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	7	0.16
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	7	0.16
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	7	0.16
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	7	0.16
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	7	0.16
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	7	0.16
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	7	0.16
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	7	0.16
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	7	0.16
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	7	0.16
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB2	4	0.16
(1,1446)	1:89:A:GLY:H	1:163:A:LEU:HB3	4	0.16
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG2	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG3	3	0.16
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG2	3	0.16
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG3	3	0.16
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG2	3	0.16
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG3	3	0.16
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG2	3	0.16
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG3	3	0.16
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG2	3	0.16
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG3	3	0.16
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG2	3	0.16
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG3	3	0.16
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	4	0.16
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	4	0.16
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	4	0.16
(1,1077)	1:70:A:VAL:HG11	1:71:A:THR:H	7	0.16
(1,1077)	1:70:A:VAL:HG12	1:71:A:THR:H	7	0.16
(1,1077)	1:70:A:VAL:HG13	1:71:A:THR:H	7	0.16
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG2	9	0.16
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG3	9	0.16
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD2	1	0.16
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD3	1	0.16
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD2	2	0.16
(1,943)	1:167:A:LYS:H	1:169:A:LYS:HD3	2	0.16
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB1	5	0.16
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB2	5	0.16
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB3	5	0.16
(1,742)	1:131:A:ILE:HD11	1:132:A:GLY:H	9	0.16
(1,742)	1:131:A:ILE:HD12	1:132:A:GLY:H	9	0.16
(1,742)	1:131:A:ILE:HD13	1:132:A:GLY:H	9	0.16
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD11	10	0.16
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD12	10	0.16
(1,729)	1:141:A:SER:HB2	1:146:A:ILE:HD13	10	0.16
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	4	0.16
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	6	0.16
(1,702)	1:47:A:ILE:HD11	1:80:A:ALA:HA	8	0.16
(1,702)	1:47:A:ILE:HD12	1:80:A:ALA:HA	8	0.16
(1,702)	1:47:A:ILE:HD13	1:80:A:ALA:HA	8	0.16
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	6	0.16
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	7	0.16
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	3	0.16
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	3	0.16
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD11	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD12	6	0.16
(1,667)	1:141:A:SER:HB3	1:146:A:ILE:HD13	6	0.16
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	5	0.16
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	6	0.16
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	3	0.16
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	3	0.16
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	3	0.16
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	3	0.16
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	3	0.16
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	3	0.16
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	3	0.16
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	3	0.16
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	3	0.16
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	5	0.16
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	5	0.16
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	5	0.16
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	5	0.16
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	5	0.16
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	5	0.16
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	5	0.16
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	5	0.16
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	5	0.16
(1,642)	1:38:A:LYS:HB2	1:39:A:ASP:HA	10	0.16
(1,642)	1:38:A:LYS:HB3	1:39:A:ASP:HA	10	0.16
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	3	0.16
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	3	0.16
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	3	0.16
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD2	7	0.16
(1,580)	1:164:A:LYS:HA	1:164:A:LYS:HD3	7	0.16
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD11	3	0.16
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD12	3	0.16
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD13	3	0.16
(1,531)	1:103:A:LYS:HG2	1:149:A:ALA:HB1	5	0.16
(1,531)	1:103:A:LYS:HG2	1:149:A:ALA:HB2	5	0.16
(1,531)	1:103:A:LYS:HG2	1:149:A:ALA:HB3	5	0.16
(1,531)	1:103:A:LYS:HG3	1:149:A:ALA:HB1	5	0.16
(1,531)	1:103:A:LYS:HG3	1:149:A:ALA:HB2	5	0.16
(1,531)	1:103:A:LYS:HG3	1:149:A:ALA:HB3	5	0.16
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	1	0.16
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	1	0.16
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	1	0.16
(1,499)	1:114:A:MET:HE1	1:156:A:LYS:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:114:A:MET:HE2	1:156:A:LYS:H	5	0.16
(1,499)	1:114:A:MET:HE3	1:156:A:LYS:H	5	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	1	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	1	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	1	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	2	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	2	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	2	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	4	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	4	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	4	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	10	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	10	0.16
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	10	0.16
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE1	4	0.16
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE2	4	0.16
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE3	4	0.16
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE1	4	0.16
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE2	4	0.16
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE3	4	0.16
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE1	4	0.16
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE2	4	0.16
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE3	4	0.16
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	7	0.16
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	7	0.16
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	7	0.16
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	8	0.16
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	8	0.16
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	8	0.16
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD21	3	0.16
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD22	3	0.16
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD23	3	0.16
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	7	0.16
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	7	0.16
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	9	0.16
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	9	0.16
(1,195)	1:155:A:ALA:HB1	1:158:A:GLN:HB2	3	0.16
(1,195)	1:155:A:ALA:HB1	1:158:A:GLN:HB3	3	0.16
(1,195)	1:155:A:ALA:HB2	1:158:A:GLN:HB2	3	0.16
(1,195)	1:155:A:ALA:HB2	1:158:A:GLN:HB3	3	0.16
(1,195)	1:155:A:ALA:HB3	1:158:A:GLN:HB2	3	0.16
(1,195)	1:155:A:ALA:HB3	1:158:A:GLN:HB3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:49:A:LYS:HB2	1:52:A:THR:HB	10	0.16
(1,132)	1:49:A:LYS:HB3	1:52:A:THR:HB	10	0.16
(1,93)	1:139:A:GLU:H	1:139:A:GLU:HG2	9	0.16
(1,93)	1:139:A:GLU:H	1:139:A:GLU:HG3	9	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG21	2	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG22	2	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG23	2	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG21	2	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG22	2	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG23	2	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG21	5	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG22	5	0.16
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG23	5	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG21	5	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG22	5	0.16
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG23	5	0.16
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD2	9	0.16
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD3	9	0.16
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE2	10	0.16
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE3	10	0.16
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE2	10	0.16
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE3	10	0.16
(1,75)	1:59:A:GLU:HA	1:59:A:GLU:HG2	9	0.16
(1,75)	1:59:A:GLU:HA	1:59:A:GLU:HG3	9	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	1	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	1	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	3	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	3	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	5	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	5	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	8	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	8	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	9	0.16
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	9	0.16
(1,1677)	1:162:A:GLN:HG2	1:165:A:VAL:HG11	10	0.15
(1,1677)	1:162:A:GLN:HG2	1:165:A:VAL:HG12	10	0.15
(1,1677)	1:162:A:GLN:HG2	1:165:A:VAL:HG13	10	0.15
(1,1677)	1:162:A:GLN:HG2	1:165:A:VAL:HG21	10	0.15
(1,1677)	1:162:A:GLN:HG2	1:165:A:VAL:HG22	10	0.15
(1,1677)	1:162:A:GLN:HG2	1:165:A:VAL:HG23	10	0.15
(1,1677)	1:162:A:GLN:HG3	1:165:A:VAL:HG11	10	0.15
(1,1677)	1:162:A:GLN:HG3	1:165:A:VAL:HG12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1677)	1:162:A:GLN:HG3	1:165:A:VAL:HG13	10	0.15
(1,1677)	1:162:A:GLN:HG3	1:165:A:VAL:HG21	10	0.15
(1,1677)	1:162:A:GLN:HG3	1:165:A:VAL:HG22	10	0.15
(1,1677)	1:162:A:GLN:HG3	1:165:A:VAL:HG23	10	0.15
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	7	0.15
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	7	0.15
(1,1564)	1:122:A:VAL:HG11	1:134:A:LYS:HE2	1	0.15
(1,1564)	1:122:A:VAL:HG11	1:134:A:LYS:HE3	1	0.15
(1,1564)	1:122:A:VAL:HG12	1:134:A:LYS:HE2	1	0.15
(1,1564)	1:122:A:VAL:HG12	1:134:A:LYS:HE3	1	0.15
(1,1564)	1:122:A:VAL:HG13	1:134:A:LYS:HE2	1	0.15
(1,1564)	1:122:A:VAL:HG13	1:134:A:LYS:HE3	1	0.15
(1,1564)	1:122:A:VAL:HG21	1:134:A:LYS:HE2	1	0.15
(1,1564)	1:122:A:VAL:HG21	1:134:A:LYS:HE3	1	0.15
(1,1564)	1:122:A:VAL:HG22	1:134:A:LYS:HE2	1	0.15
(1,1564)	1:122:A:VAL:HG22	1:134:A:LYS:HE3	1	0.15
(1,1564)	1:122:A:VAL:HG23	1:134:A:LYS:HE2	1	0.15
(1,1564)	1:122:A:VAL:HG23	1:134:A:LYS:HE3	1	0.15
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	2	0.15
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	2	0.15
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	2	0.15
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	2	0.15
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	2	0.15
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	2	0.15
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	2	0.15
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	2	0.15
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	2	0.15
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	2	0.15
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	2	0.15
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	2	0.15
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	2	0.15
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	2	0.15
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	2	0.15
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	2	0.15
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	2	0.15
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	2	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD11	2	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD12	2	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD13	2	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD21	2	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD22	2	0.15
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD23	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD11	2	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD12	2	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD13	2	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD21	2	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD22	2	0.15
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD23	2	0.15
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD11	5	0.15
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD12	5	0.15
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD13	5	0.15
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD21	5	0.15
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD22	5	0.15
(1,1445)	1:89:A:GLY:H	1:92:A:LEU:HD23	5	0.15
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG12	9	0.15
(1,1415)	1:82:A:VAL:HG11	1:85:A:ILE:HG13	9	0.15
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG12	9	0.15
(1,1415)	1:82:A:VAL:HG12	1:85:A:ILE:HG13	9	0.15
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG12	9	0.15
(1,1415)	1:82:A:VAL:HG13	1:85:A:ILE:HG13	9	0.15
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG12	9	0.15
(1,1415)	1:82:A:VAL:HG21	1:85:A:ILE:HG13	9	0.15
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG12	9	0.15
(1,1415)	1:82:A:VAL:HG22	1:85:A:ILE:HG13	9	0.15
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG12	9	0.15
(1,1415)	1:82:A:VAL:HG23	1:85:A:ILE:HG13	9	0.15
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG11	10	0.15
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG12	10	0.15
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG13	10	0.15
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG21	10	0.15
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG22	10	0.15
(1,1391)	1:69:A:LYS:HA	1:70:A:VAL:HG23	10	0.15
(1,1312)	1:40:A:LEU:HD11	1:125:A:LEU:H	1	0.15
(1,1312)	1:40:A:LEU:HD12	1:125:A:LEU:H	1	0.15
(1,1312)	1:40:A:LEU:HD13	1:125:A:LEU:H	1	0.15
(1,1312)	1:40:A:LEU:HD21	1:125:A:LEU:H	1	0.15
(1,1312)	1:40:A:LEU:HD22	1:125:A:LEU:H	1	0.15
(1,1312)	1:40:A:LEU:HD23	1:125:A:LEU:H	1	0.15
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB2	8	0.15
(1,1294)	1:40:A:LEU:HD11	1:41:A:LYS:HB3	8	0.15
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB2	8	0.15
(1,1294)	1:40:A:LEU:HD12	1:41:A:LYS:HB3	8	0.15
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB2	8	0.15
(1,1294)	1:40:A:LEU:HD13	1:41:A:LYS:HB3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB2	8	0.15
(1,1294)	1:40:A:LEU:HD21	1:41:A:LYS:HB3	8	0.15
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB2	8	0.15
(1,1294)	1:40:A:LEU:HD22	1:41:A:LYS:HB3	8	0.15
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB2	8	0.15
(1,1294)	1:40:A:LEU:HD23	1:41:A:LYS:HB3	8	0.15
(1,1268)	1:33:A:LEU:HD11	1:95:A:ILE:HG21	7	0.15
(1,1268)	1:33:A:LEU:HD11	1:95:A:ILE:HG22	7	0.15
(1,1268)	1:33:A:LEU:HD11	1:95:A:ILE:HG23	7	0.15
(1,1268)	1:33:A:LEU:HD12	1:95:A:ILE:HG21	7	0.15
(1,1268)	1:33:A:LEU:HD12	1:95:A:ILE:HG22	7	0.15
(1,1268)	1:33:A:LEU:HD12	1:95:A:ILE:HG23	7	0.15
(1,1268)	1:33:A:LEU:HD13	1:95:A:ILE:HG21	7	0.15
(1,1268)	1:33:A:LEU:HD13	1:95:A:ILE:HG22	7	0.15
(1,1268)	1:33:A:LEU:HD13	1:95:A:ILE:HG23	7	0.15
(1,1268)	1:33:A:LEU:HD21	1:95:A:ILE:HG21	7	0.15
(1,1268)	1:33:A:LEU:HD21	1:95:A:ILE:HG22	7	0.15
(1,1268)	1:33:A:LEU:HD21	1:95:A:ILE:HG23	7	0.15
(1,1268)	1:33:A:LEU:HD22	1:95:A:ILE:HG21	7	0.15
(1,1268)	1:33:A:LEU:HD22	1:95:A:ILE:HG22	7	0.15
(1,1268)	1:33:A:LEU:HD22	1:95:A:ILE:HG23	7	0.15
(1,1268)	1:33:A:LEU:HD23	1:95:A:ILE:HG21	7	0.15
(1,1268)	1:33:A:LEU:HD23	1:95:A:ILE:HG22	7	0.15
(1,1268)	1:33:A:LEU:HD23	1:95:A:ILE:HG23	7	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD11	1	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD12	1	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD13	1	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD21	1	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD22	1	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD23	1	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD11	1	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD12	1	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD13	1	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD21	1	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD22	1	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD23	1	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD11	1	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD12	1	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD13	1	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD21	1	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD22	1	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD23	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD11	3	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD12	3	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD13	3	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD21	3	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD22	3	0.15
(1,1253)	1:32:A:ALA:HB1	1:33:A:LEU:HD23	3	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD11	3	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD12	3	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD13	3	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD21	3	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD22	3	0.15
(1,1253)	1:32:A:ALA:HB2	1:33:A:LEU:HD23	3	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD11	3	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD12	3	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD13	3	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD21	3	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD22	3	0.15
(1,1253)	1:32:A:ALA:HB3	1:33:A:LEU:HD23	3	0.15
(1,1195)	1:111:A:PHE:H	1:147:A:ASN:HA	6	0.15
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD11	5	0.15
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD12	5	0.15
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD13	5	0.15
(1,1115)	1:103:A:LYS:HG2	1:150:A:GLU:H	5	0.15
(1,1115)	1:103:A:LYS:HG3	1:150:A:GLU:H	5	0.15
(1,1041)	1:159:A:ILE:HB	1:162:A:GLN:H	3	0.15
(1,886)	1:146:A:ILE:HG21	1:149:A:ALA:H	7	0.15
(1,886)	1:146:A:ILE:HG22	1:149:A:ALA:H	7	0.15
(1,886)	1:146:A:ILE:HG23	1:149:A:ALA:H	7	0.15
(1,796)	1:99:A:ALA:HB1	1:111:A:PHE:HD1	5	0.15
(1,796)	1:99:A:ALA:HB1	1:111:A:PHE:HD2	5	0.15
(1,796)	1:99:A:ALA:HB2	1:111:A:PHE:HD1	5	0.15
(1,796)	1:99:A:ALA:HB2	1:111:A:PHE:HD2	5	0.15
(1,796)	1:99:A:ALA:HB3	1:111:A:PHE:HD1	5	0.15
(1,796)	1:99:A:ALA:HB3	1:111:A:PHE:HD2	5	0.15
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB1	4	0.15
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB2	4	0.15
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB3	4	0.15
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB1	4	0.15
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB2	4	0.15
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB3	4	0.15
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	1	0.15
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:41:A:LYS:H	1:41:A:LYS:HD2	6	0.15
(1,712)	1:41:A:LYS:H	1:41:A:LYS:HD3	6	0.15
(1,694)	1:114:A:MET:HE1	1:118:A:MET:HB3	9	0.15
(1,694)	1:114:A:MET:HE2	1:118:A:MET:HB3	9	0.15
(1,694)	1:114:A:MET:HE3	1:118:A:MET:HB3	9	0.15
(1,679)	1:29:A:THR:HA	1:30:A:ASN:HA	2	0.15
(1,661)	1:157:A:ALA:HA	1:159:A:ILE:H	6	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	1	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	1	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	1	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	1	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	1	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	1	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	1	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	1	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	1	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	2	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	2	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	2	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	2	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	2	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	2	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	2	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	2	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	2	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	4	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	4	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	4	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	4	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	4	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	4	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	4	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	4	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	4	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	8	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	8	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	8	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	8	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	8	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	8	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	8	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	8	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	10	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	10	0.15
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	10	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	10	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	10	0.15
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	10	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	10	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	10	0.15
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	10	0.15
(1,626)	1:25:A:LEU:HA	1:26:A:VAL:H	2	0.15
(1,626)	1:25:A:LEU:HA	1:26:A:VAL:H	7	0.15
(1,612)	1:155:A:ALA:HB1	1:159:A:ILE:HD11	3	0.15
(1,612)	1:155:A:ALA:HB1	1:159:A:ILE:HD12	3	0.15
(1,612)	1:155:A:ALA:HB1	1:159:A:ILE:HD13	3	0.15
(1,612)	1:155:A:ALA:HB2	1:159:A:ILE:HD11	3	0.15
(1,612)	1:155:A:ALA:HB2	1:159:A:ILE:HD12	3	0.15
(1,612)	1:155:A:ALA:HB2	1:159:A:ILE:HD13	3	0.15
(1,612)	1:155:A:ALA:HB3	1:159:A:ILE:HD11	3	0.15
(1,612)	1:155:A:ALA:HB3	1:159:A:ILE:HD12	3	0.15
(1,612)	1:155:A:ALA:HB3	1:159:A:ILE:HD13	3	0.15
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD11	8	0.15
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD12	8	0.15
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD13	8	0.15
(1,560)	1:126:A:GLU:HA	1:130:A:ILE:HA	2	0.15
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	4	0.15
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	4	0.15
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	4	0.15
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB1	6	0.15
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB2	6	0.15
(1,519)	1:111:A:PHE:HA	1:149:A:ALA:HB3	6	0.15
(1,502)	1:63:A:GLY:H	1:66:A:THR:HA	6	0.15
(1,502)	1:63:A:GLY:H	1:66:A:THR:HA	8	0.15
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	5	0.15
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	5	0.15
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	5	0.15
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	2	0.15
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	2	0.15
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	2	0.15
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	2	0.15
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	2	0.15
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	2	0.15
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	2	0.15
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	2	0.15
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	2	0.15
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	2	0.15
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	2	0.15
(1,358)	1:121:A:VAL:HG21	1:122:A:VAL:H	9	0.15
(1,358)	1:121:A:VAL:HG22	1:122:A:VAL:H	9	0.15
(1,358)	1:121:A:VAL:HG23	1:122:A:VAL:H	9	0.15
(1,318)	1:102:A:LEU:HD11	1:106:A:GLY:H	1	0.15
(1,318)	1:102:A:LEU:HD12	1:106:A:GLY:H	1	0.15
(1,318)	1:102:A:LEU:HD13	1:106:A:GLY:H	1	0.15
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	4	0.15
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	4	0.15
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG2	2	0.15
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG3	2	0.15
(1,174)	1:65:A:LYS:HA	1:65:A:LYS:HD2	8	0.15
(1,174)	1:65:A:LYS:HA	1:65:A:LYS:HD3	8	0.15
(1,154)	1:81:A:LYS:HD2	1:128:A:VAL:HB	1	0.15
(1,154)	1:81:A:LYS:HD3	1:128:A:VAL:HB	1	0.15
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG21	4	0.15
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG22	4	0.15
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG23	4	0.15
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG21	4	0.15
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG22	4	0.15
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG23	4	0.15
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG21	10	0.15
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG22	10	0.15
(1,91)	1:104:A:GLU:HG2	1:105:A:THR:HG23	10	0.15
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG21	10	0.15
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG22	10	0.15
(1,91)	1:104:A:GLU:HG3	1:105:A:THR:HG23	10	0.15
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	3	0.15
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	3	0.15
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	3	0.15
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	3	0.15
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	3	0.15
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	3	0.15
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG2	5	0.15
(1,88)	1:136:A:ARG:HG2	1:139:A:GLU:HG3	5	0.15
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG2	5	0.15
(1,88)	1:136:A:ARG:HG3	1:139:A:GLU:HG3	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:160:A:GLU:H	1:160:A:GLU:HG2	9	0.15
(1,6)	1:28:A:ARG:HD2	1:29:A:THR:H	8	0.15
(1,6)	1:28:A:ARG:HD3	1:29:A:THR:H	8	0.15
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG21	4	0.14
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG22	4	0.14
(1,1618)	1:137:A:VAL:HG11	1:159:A:ILE:HG23	4	0.14
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG21	4	0.14
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG22	4	0.14
(1,1618)	1:137:A:VAL:HG12	1:159:A:ILE:HG23	4	0.14
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG21	4	0.14
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG22	4	0.14
(1,1618)	1:137:A:VAL:HG13	1:159:A:ILE:HG23	4	0.14
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG21	4	0.14
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG22	4	0.14
(1,1618)	1:137:A:VAL:HG21	1:159:A:ILE:HG23	4	0.14
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG21	4	0.14
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG22	4	0.14
(1,1618)	1:137:A:VAL:HG22	1:159:A:ILE:HG23	4	0.14
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG21	4	0.14
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG22	4	0.14
(1,1618)	1:137:A:VAL:HG23	1:159:A:ILE:HG23	4	0.14
(1,1591)	1:133:A:LEU:HD11	1:163:A:LEU:HA	6	0.14
(1,1591)	1:133:A:LEU:HD12	1:163:A:LEU:HA	6	0.14
(1,1591)	1:133:A:LEU:HD13	1:163:A:LEU:HA	6	0.14
(1,1591)	1:133:A:LEU:HD21	1:163:A:LEU:HA	6	0.14
(1,1591)	1:133:A:LEU:HD22	1:163:A:LEU:HA	6	0.14
(1,1591)	1:133:A:LEU:HD23	1:163:A:LEU:HA	6	0.14
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	10	0.14
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	10	0.14
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	10	0.14
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	10	0.14
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	10	0.14
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	10	0.14
(1,1529)	1:116:A:ASP:HA	1:119:A:LEU:HD11	5	0.14
(1,1529)	1:116:A:ASP:HA	1:119:A:LEU:HD12	5	0.14
(1,1529)	1:116:A:ASP:HA	1:119:A:LEU:HD13	5	0.14
(1,1529)	1:116:A:ASP:HA	1:119:A:LEU:HD21	5	0.14
(1,1529)	1:116:A:ASP:HA	1:119:A:LEU:HD22	5	0.14
(1,1529)	1:116:A:ASP:HA	1:119:A:LEU:HD23	5	0.14
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB1	6	0.14
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB2	6	0.14
(1,1494)	1:102:A:LEU:HD11	1:149:A:ALA:HB3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB1	6	0.14
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB2	6	0.14
(1,1494)	1:102:A:LEU:HD12	1:149:A:ALA:HB3	6	0.14
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB1	6	0.14
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB2	6	0.14
(1,1494)	1:102:A:LEU:HD13	1:149:A:ALA:HB3	6	0.14
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	6	0.14
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	6	0.14
(1,1494)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	6	0.14
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	6	0.14
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	6	0.14
(1,1494)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	6	0.14
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	6	0.14
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	6	0.14
(1,1494)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	6	0.14
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG2	6	0.14
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG3	6	0.14
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG2	6	0.14
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG3	6	0.14
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG2	6	0.14
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG3	6	0.14
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG2	6	0.14
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG3	6	0.14
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG2	6	0.14
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG3	6	0.14
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG2	6	0.14
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG3	6	0.14
(1,1411)	1:82:A:VAL:HB	1:170:A:GLN:HG2	3	0.14
(1,1411)	1:82:A:VAL:HB	1:170:A:GLN:HG3	3	0.14
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD11	2	0.14
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD12	2	0.14
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD13	2	0.14
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD21	2	0.14
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD22	2	0.14
(1,1337)	1:45:A:LEU:HA	1:45:A:LEU:HD23	2	0.14
(1,1299)	1:40:A:LEU:HD11	1:44:A:ILE:HD11	3	0.14
(1,1299)	1:40:A:LEU:HD11	1:44:A:ILE:HD12	3	0.14
(1,1299)	1:40:A:LEU:HD11	1:44:A:ILE:HD13	3	0.14
(1,1299)	1:40:A:LEU:HD12	1:44:A:ILE:HD11	3	0.14
(1,1299)	1:40:A:LEU:HD12	1:44:A:ILE:HD12	3	0.14
(1,1299)	1:40:A:LEU:HD12	1:44:A:ILE:HD13	3	0.14
(1,1299)	1:40:A:LEU:HD13	1:44:A:ILE:HD11	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1299)	1:40:A:LEU:HD13	1:44:A:ILE:HD12	3	0.14
(1,1299)	1:40:A:LEU:HD13	1:44:A:ILE:HD13	3	0.14
(1,1299)	1:40:A:LEU:HD21	1:44:A:ILE:HD11	3	0.14
(1,1299)	1:40:A:LEU:HD21	1:44:A:ILE:HD12	3	0.14
(1,1299)	1:40:A:LEU:HD21	1:44:A:ILE:HD13	3	0.14
(1,1299)	1:40:A:LEU:HD22	1:44:A:ILE:HD11	3	0.14
(1,1299)	1:40:A:LEU:HD22	1:44:A:ILE:HD12	3	0.14
(1,1299)	1:40:A:LEU:HD22	1:44:A:ILE:HD13	3	0.14
(1,1299)	1:40:A:LEU:HD23	1:44:A:ILE:HD11	3	0.14
(1,1299)	1:40:A:LEU:HD23	1:44:A:ILE:HD12	3	0.14
(1,1299)	1:40:A:LEU:HD23	1:44:A:ILE:HD13	3	0.14
(1,1272)	1:34:A:GLU:H	1:34:A:GLU:HG2	6	0.14
(1,1272)	1:34:A:GLU:H	1:34:A:GLU:HG3	6	0.14
(1,1249)	1:30:A:ASN:HD21	1:32:A:ALA:HB1	10	0.14
(1,1249)	1:30:A:ASN:HD21	1:32:A:ALA:HB2	10	0.14
(1,1249)	1:30:A:ASN:HD21	1:32:A:ALA:HB3	10	0.14
(1,1249)	1:30:A:ASN:HD22	1:32:A:ALA:HB1	10	0.14
(1,1249)	1:30:A:ASN:HD22	1:32:A:ALA:HB2	10	0.14
(1,1249)	1:30:A:ASN:HD22	1:32:A:ALA:HB3	10	0.14
(1,1248)	1:30:A:ASN:HD21	1:31:A:ALA:HB1	5	0.14
(1,1248)	1:30:A:ASN:HD21	1:31:A:ALA:HB2	5	0.14
(1,1248)	1:30:A:ASN:HD21	1:31:A:ALA:HB3	5	0.14
(1,1248)	1:30:A:ASN:HD22	1:31:A:ALA:HB1	5	0.14
(1,1248)	1:30:A:ASN:HD22	1:31:A:ALA:HB2	5	0.14
(1,1248)	1:30:A:ASN:HD22	1:31:A:ALA:HB3	5	0.14
(1,1209)	1:64:A:LEU:HD21	1:67:A:GLY:H	2	0.14
(1,1209)	1:64:A:LEU:HD22	1:67:A:GLY:H	2	0.14
(1,1209)	1:64:A:LEU:HD23	1:67:A:GLY:H	2	0.14
(1,1147)	1:139:A:GLU:HG2	1:141:A:SER:H	6	0.14
(1,1147)	1:139:A:GLU:HG3	1:141:A:SER:H	6	0.14
(1,1147)	1:139:A:GLU:HG2	1:141:A:SER:H	7	0.14
(1,1147)	1:139:A:GLU:HG3	1:141:A:SER:H	7	0.14
(1,1140)	1:35:A:SER:H	1:38:A:LYS:HG2	7	0.14
(1,1140)	1:35:A:SER:H	1:38:A:LYS:HG3	7	0.14
(1,1131)	1:33:A:LEU:HD21	1:97:A:GLU:H	10	0.14
(1,1131)	1:33:A:LEU:HD22	1:97:A:GLU:H	10	0.14
(1,1131)	1:33:A:LEU:HD23	1:97:A:GLU:H	10	0.14
(1,1129)	1:101:A:LYS:HD2	1:102:A:LEU:H	5	0.14
(1,1129)	1:101:A:LYS:HD3	1:102:A:LEU:H	5	0.14
(1,1116)	1:101:A:LYS:HD2	1:104:A:GLU:H	7	0.14
(1,1116)	1:101:A:LYS:HD3	1:104:A:GLU:H	7	0.14
(1,886)	1:146:A:ILE:HG21	1:149:A:ALA:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:146:A:ILE:HG22	1:149:A:ALA:H	8	0.14
(1,886)	1:146:A:ILE:HG23	1:149:A:ALA:H	8	0.14
(1,803)	1:146:A:ILE:HD11	1:151:A:ARG:HD2	4	0.14
(1,803)	1:146:A:ILE:HD11	1:151:A:ARG:HD3	4	0.14
(1,803)	1:146:A:ILE:HD12	1:151:A:ARG:HD2	4	0.14
(1,803)	1:146:A:ILE:HD12	1:151:A:ARG:HD3	4	0.14
(1,803)	1:146:A:ILE:HD13	1:151:A:ARG:HD2	4	0.14
(1,803)	1:146:A:ILE:HD13	1:151:A:ARG:HD3	4	0.14
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD11	7	0.14
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD12	7	0.14
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD13	7	0.14
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD11	7	0.14
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD12	7	0.14
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD13	7	0.14
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB1	5	0.14
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB2	5	0.14
(1,784)	1:103:A:LYS:HE2	1:149:A:ALA:HB3	5	0.14
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB1	5	0.14
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB2	5	0.14
(1,784)	1:103:A:LYS:HE3	1:149:A:ALA:HB3	5	0.14
(1,755)	1:44:A:ILE:HD11	1:124:A:SER:H	4	0.14
(1,755)	1:44:A:ILE:HD12	1:124:A:SER:H	4	0.14
(1,755)	1:44:A:ILE:HD13	1:124:A:SER:H	4	0.14
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	3	0.14
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	7	0.14
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	9	0.14
(1,699)	1:45:A:LEU:HG	1:46:A:LYS:HA	3	0.14
(1,694)	1:114:A:MET:HE1	1:118:A:MET:HB3	8	0.14
(1,694)	1:114:A:MET:HE2	1:118:A:MET:HB3	8	0.14
(1,694)	1:114:A:MET:HE3	1:118:A:MET:HB3	8	0.14
(1,673)	1:80:A:ALA:HA	1:83:A:GLN:HB3	9	0.14
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	10	0.14
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	6	0.14
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	6	0.14
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	6	0.14
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	6	0.14
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	6	0.14
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	6	0.14
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	6	0.14
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	6	0.14
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	6	0.14
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD11	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD12	9	0.14
(1,657)	1:44:A:ILE:HG21	1:44:A:ILE:HD13	9	0.14
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD11	9	0.14
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD12	9	0.14
(1,657)	1:44:A:ILE:HG22	1:44:A:ILE:HD13	9	0.14
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD11	9	0.14
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD12	9	0.14
(1,657)	1:44:A:ILE:HG23	1:44:A:ILE:HD13	9	0.14
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	10	0.14
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	7	0.14
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	7	0.14
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	7	0.14
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	7	0.14
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	7	0.14
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	7	0.14
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	7	0.14
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	7	0.14
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	7	0.14
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB1	10	0.14
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB2	10	0.14
(1,539)	1:102:A:LEU:HD21	1:149:A:ALA:HB3	10	0.14
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB1	10	0.14
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB2	10	0.14
(1,539)	1:102:A:LEU:HD22	1:149:A:ALA:HB3	10	0.14
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB1	10	0.14
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB2	10	0.14
(1,539)	1:102:A:LEU:HD23	1:149:A:ALA:HB3	10	0.14
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE1	2	0.14
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE2	2	0.14
(1,476)	1:99:A:ALA:HB1	1:118:A:MET:HE3	2	0.14
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE1	2	0.14
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE2	2	0.14
(1,476)	1:99:A:ALA:HB2	1:118:A:MET:HE3	2	0.14
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE1	2	0.14
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE2	2	0.14
(1,476)	1:99:A:ALA:HB3	1:118:A:MET:HE3	2	0.14
(1,455)	1:129:A:GLY:HA2	1:131:A:ILE:HG21	5	0.14
(1,455)	1:129:A:GLY:HA2	1:131:A:ILE:HG22	5	0.14
(1,455)	1:129:A:GLY:HA2	1:131:A:ILE:HG23	5	0.14
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	6	0.14
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	6	0.14
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	4	0.14
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	4	0.14
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	4	0.14
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG11	8	0.14
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG12	8	0.14
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG13	8	0.14
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD21	1	0.14
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD22	1	0.14
(1,298)	1:64:A:LEU:HA	1:64:A:LEU:HD23	1	0.14
(1,242)	1:133:A:LEU:H	1:133:A:LEU:HD11	5	0.14
(1,242)	1:133:A:LEU:H	1:133:A:LEU:HD12	5	0.14
(1,242)	1:133:A:LEU:H	1:133:A:LEU:HD13	5	0.14
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	1	0.14
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	1	0.14
(1,218)	1:109:A:GLY:HA2	1:112:A:LEU:HG	8	0.14
(1,218)	1:109:A:GLY:HA3	1:112:A:LEU:HG	8	0.14
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD21	5	0.14
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD22	5	0.14
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD23	5	0.14
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD21	5	0.14
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD22	5	0.14
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD23	5	0.14
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD21	5	0.14
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD22	5	0.14
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD23	5	0.14
(1,134)	1:44:A:ILE:HA	1:48:A:LYS:HB2	7	0.14
(1,134)	1:44:A:ILE:HA	1:48:A:LYS:HB3	7	0.14
(1,101)	1:83:A:GLN:H	1:83:A:GLN:HG3	3	0.14
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	4	0.14
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	4	0.14
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	8	0.14
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	8	0.14
(1,1699)	1:172:A:ILE:HG12	1:173:A:GLU:HG2	5	0.13
(1,1699)	1:172:A:ILE:HG12	1:173:A:GLU:HG3	5	0.13
(1,1699)	1:172:A:ILE:HG13	1:173:A:GLU:HG2	5	0.13
(1,1699)	1:172:A:ILE:HG13	1:173:A:GLU:HG3	5	0.13
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD11	10	0.13
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD12	10	0.13
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD13	10	0.13
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD21	10	0.13
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD22	10	0.13
(1,1645)	1:150:A:GLU:HA	1:153:A:LEU:HD23	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1625)	1:139:A:GLU:HB2	1:142:A:LYS:HE2	9	0.13
(1,1625)	1:139:A:GLU:HB2	1:142:A:LYS:HE3	9	0.13
(1,1625)	1:139:A:GLU:HB3	1:142:A:LYS:HE2	9	0.13
(1,1625)	1:139:A:GLU:HB3	1:142:A:LYS:HE3	9	0.13
(1,1587)	1:133:A:LEU:HD11	1:162:A:GLN:H	8	0.13
(1,1587)	1:133:A:LEU:HD12	1:162:A:GLN:H	8	0.13
(1,1587)	1:133:A:LEU:HD13	1:162:A:GLN:H	8	0.13
(1,1587)	1:133:A:LEU:HD21	1:162:A:GLN:H	8	0.13
(1,1587)	1:133:A:LEU:HD22	1:162:A:GLN:H	8	0.13
(1,1587)	1:133:A:LEU:HD23	1:162:A:GLN:H	8	0.13
(1,1562)	1:122:A:VAL:HG11	1:134:A:LYS:HB2	2	0.13
(1,1562)	1:122:A:VAL:HG11	1:134:A:LYS:HB3	2	0.13
(1,1562)	1:122:A:VAL:HG12	1:134:A:LYS:HB2	2	0.13
(1,1562)	1:122:A:VAL:HG12	1:134:A:LYS:HB3	2	0.13
(1,1562)	1:122:A:VAL:HG13	1:134:A:LYS:HB2	2	0.13
(1,1562)	1:122:A:VAL:HG13	1:134:A:LYS:HB3	2	0.13
(1,1562)	1:122:A:VAL:HG21	1:134:A:LYS:HB2	2	0.13
(1,1562)	1:122:A:VAL:HG21	1:134:A:LYS:HB3	2	0.13
(1,1562)	1:122:A:VAL:HG22	1:134:A:LYS:HB2	2	0.13
(1,1562)	1:122:A:VAL:HG22	1:134:A:LYS:HB3	2	0.13
(1,1562)	1:122:A:VAL:HG23	1:134:A:LYS:HB2	2	0.13
(1,1562)	1:122:A:VAL:HG23	1:134:A:LYS:HB3	2	0.13
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG11	3	0.13
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG12	3	0.13
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG13	3	0.13
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG21	3	0.13
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG22	3	0.13
(1,1545)	1:119:A:LEU:HB2	1:122:A:VAL:HG23	3	0.13
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	3	0.13
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	3	0.13
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	3	0.13
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	3	0.13
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	3	0.13
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	3	0.13
(1,1490)	1:102:A:LEU:HD11	1:110:A:GLN:HE21	4	0.13
(1,1490)	1:102:A:LEU:HD11	1:110:A:GLN:HE22	4	0.13
(1,1490)	1:102:A:LEU:HD12	1:110:A:GLN:HE21	4	0.13
(1,1490)	1:102:A:LEU:HD12	1:110:A:GLN:HE22	4	0.13
(1,1490)	1:102:A:LEU:HD13	1:110:A:GLN:HE21	4	0.13
(1,1490)	1:102:A:LEU:HD13	1:110:A:GLN:HE22	4	0.13
(1,1490)	1:102:A:LEU:HD21	1:110:A:GLN:HE21	4	0.13
(1,1490)	1:102:A:LEU:HD21	1:110:A:GLN:HE22	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:102:A:LEU:HD22	1:110:A:GLN:HE21	4	0.13
(1,1490)	1:102:A:LEU:HD22	1:110:A:GLN:HE22	4	0.13
(1,1490)	1:102:A:LEU:HD23	1:110:A:GLN:HE21	4	0.13
(1,1490)	1:102:A:LEU:HD23	1:110:A:GLN:HE22	4	0.13
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG2	4	0.13
(1,1456)	1:92:A:LEU:HD11	1:96:A:GLU:HG3	4	0.13
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG2	4	0.13
(1,1456)	1:92:A:LEU:HD12	1:96:A:GLU:HG3	4	0.13
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG2	4	0.13
(1,1456)	1:92:A:LEU:HD13	1:96:A:GLU:HG3	4	0.13
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG2	4	0.13
(1,1456)	1:92:A:LEU:HD21	1:96:A:GLU:HG3	4	0.13
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG2	4	0.13
(1,1456)	1:92:A:LEU:HD22	1:96:A:GLU:HG3	4	0.13
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG2	4	0.13
(1,1456)	1:92:A:LEU:HD23	1:96:A:GLU:HG3	4	0.13
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG11	9	0.13
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG12	9	0.13
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG13	9	0.13
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG21	9	0.13
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG22	9	0.13
(1,1392)	1:69:A:LYS:HG2	1:70:A:VAL:HG23	9	0.13
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG11	9	0.13
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG12	9	0.13
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG13	9	0.13
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG21	9	0.13
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG22	9	0.13
(1,1392)	1:69:A:LYS:HG3	1:70:A:VAL:HG23	9	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD11	1	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD12	1	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD13	1	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD21	1	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD22	1	0.13
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD23	1	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD11	1	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD12	1	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD13	1	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD21	1	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD22	1	0.13
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD23	1	0.13
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB2	3	0.13
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD11	3	0.13
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD12	3	0.13
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD13	3	0.13
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD21	3	0.13
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD22	3	0.13
(1,1329)	1:43:A:LYS:HE2	1:45:A:LEU:HD23	3	0.13
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD11	3	0.13
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD12	3	0.13
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD13	3	0.13
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD21	3	0.13
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD22	3	0.13
(1,1329)	1:43:A:LYS:HE3	1:45:A:LEU:HD23	3	0.13
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD11	3	0.13
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD12	3	0.13
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD13	3	0.13
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD21	3	0.13
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD22	3	0.13
(1,1318)	1:41:A:LYS:HD2	1:117:A:LEU:HD23	3	0.13
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD11	3	0.13
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD12	3	0.13
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD13	3	0.13
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD21	3	0.13
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD22	3	0.13
(1,1318)	1:41:A:LYS:HD3	1:117:A:LEU:HD23	3	0.13
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG21	7	0.13
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG22	7	0.13
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG23	7	0.13
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG21	7	0.13
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG22	7	0.13
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG23	7	0.13
(1,1272)	1:34:A:GLU:H	1:34:A:GLU:HG2	4	0.13
(1,1272)	1:34:A:GLU:H	1:34:A:GLU:HG3	4	0.13
(1,1219)	1:146:A:ILE:HD11	1:149:A:ALA:H	10	0.13
(1,1219)	1:146:A:ILE:HD12	1:149:A:ALA:H	10	0.13
(1,1219)	1:146:A:ILE:HD13	1:149:A:ALA:H	10	0.13
(1,1192)	1:146:A:ILE:H	1:148:A:THR:H	7	0.13
(1,1189)	1:144:A:ASN:H	1:146:A:ILE:HD11	6	0.13
(1,1189)	1:144:A:ASN:H	1:146:A:ILE:HD12	6	0.13
(1,1189)	1:144:A:ASN:H	1:146:A:ILE:HD13	6	0.13
(1,1116)	1:101:A:LYS:HD2	1:104:A:GLU:H	5	0.13
(1,1116)	1:101:A:LYS:HD3	1:104:A:GLU:H	5	0.13
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD11	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD12	3	0.13
(1,1079)	1:137:A:VAL:H	1:159:A:ILE:HD13	3	0.13
(1,1051)	1:38:A:LYS:HD2	1:39:A:ASP:H	4	0.13
(1,1051)	1:38:A:LYS:HD3	1:39:A:ASP:H	4	0.13
(1,1042)	1:121:A:VAL:HB	1:124:A:SER:H	10	0.13
(1,975)	1:115:A:PHE:H	1:146:A:ILE:HG21	7	0.13
(1,975)	1:115:A:PHE:H	1:146:A:ILE:HG22	7	0.13
(1,975)	1:115:A:PHE:H	1:146:A:ILE:HG23	7	0.13
(1,883)	1:23:A:ILE:HG21	1:25:A:LEU:H	10	0.13
(1,883)	1:23:A:ILE:HG22	1:25:A:LEU:H	10	0.13
(1,883)	1:23:A:ILE:HG23	1:25:A:LEU:H	10	0.13
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD11	8	0.13
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD12	8	0.13
(1,800)	1:91:A:PHE:HE1	1:117:A:LEU:HD13	8	0.13
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD11	8	0.13
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD12	8	0.13
(1,800)	1:91:A:PHE:HE2	1:117:A:LEU:HD13	8	0.13
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB1	10	0.13
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB2	10	0.13
(1,788)	1:111:A:PHE:H	1:113:A:ALA:HB3	10	0.13
(1,755)	1:44:A:ILE:HD11	1:124:A:SER:H	1	0.13
(1,755)	1:44:A:ILE:HD12	1:124:A:SER:H	1	0.13
(1,755)	1:44:A:ILE:HD13	1:124:A:SER:H	1	0.13
(1,748)	1:39:A:ASP:HA	1:42:A:ASN:HD22	7	0.13
(1,726)	1:115:A:PHE:HB2	1:116:A:ASP:HA	2	0.13
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	1	0.13
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	8	0.13
(1,697)	1:103:A:LYS:HA	1:149:A:ALA:HA	9	0.13
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	1	0.13
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	1	0.13
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	6	0.13
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	6	0.13
(1,578)	1:101:A:LYS:HA	1:101:A:LYS:HD2	1	0.13
(1,578)	1:101:A:LYS:HA	1:101:A:LYS:HD3	1	0.13
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD11	3	0.13
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD12	3	0.13
(1,496)	1:95:A:ILE:HA	1:95:A:ILE:HD13	3	0.13
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	7	0.13
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	7	0.13
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	7	0.13
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	9	0.13
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	9	0.13
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG21	8	0.13
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG22	8	0.13
(1,394)	1:104:A:GLU:HB3	1:105:A:THR:HG23	8	0.13
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG11	3	0.13
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG12	3	0.13
(1,357)	1:84:A:ALA:H	1:128:A:VAL:HG13	3	0.13
(1,226)	1:40:A:LEU:HD21	1:88:A:THR:HG21	3	0.13
(1,226)	1:40:A:LEU:HD21	1:88:A:THR:HG22	3	0.13
(1,226)	1:40:A:LEU:HD21	1:88:A:THR:HG23	3	0.13
(1,226)	1:40:A:LEU:HD22	1:88:A:THR:HG21	3	0.13
(1,226)	1:40:A:LEU:HD22	1:88:A:THR:HG22	3	0.13
(1,226)	1:40:A:LEU:HD22	1:88:A:THR:HG23	3	0.13
(1,226)	1:40:A:LEU:HD23	1:88:A:THR:HG21	3	0.13
(1,226)	1:40:A:LEU:HD23	1:88:A:THR:HG22	3	0.13
(1,226)	1:40:A:LEU:HD23	1:88:A:THR:HG23	3	0.13
(1,204)	1:77:A:LEU:HG	1:81:A:LYS:H	10	0.13
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD21	8	0.13
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD22	8	0.13
(1,200)	1:146:A:ILE:HG21	1:152:A:LEU:HD23	8	0.13
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD21	8	0.13
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD22	8	0.13
(1,200)	1:146:A:ILE:HG22	1:152:A:LEU:HD23	8	0.13
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD21	8	0.13
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD22	8	0.13
(1,200)	1:146:A:ILE:HG23	1:152:A:LEU:HD23	8	0.13
(1,169)	1:139:A:GLU:H	1:140:A:GLU:HB2	7	0.13
(1,169)	1:139:A:GLU:H	1:140:A:GLU:HB3	7	0.13
(1,155)	1:51:A:ALA:HB1	1:56:A:VAL:HB	9	0.13
(1,155)	1:51:A:ALA:HB2	1:56:A:VAL:HB	9	0.13
(1,155)	1:51:A:ALA:HB3	1:56:A:VAL:HB	9	0.13
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB1	8	0.13
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB2	8	0.13
(1,89)	1:50:A:GLU:HG2	1:51:A:ALA:HB3	8	0.13
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB1	8	0.13
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB2	8	0.13
(1,89)	1:50:A:GLU:HG3	1:51:A:ALA:HB3	8	0.13
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE2	5	0.13
(1,81)	1:168:A:GLU:HG2	1:169:A:LYS:HE3	5	0.13
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE2	5	0.13
(1,81)	1:168:A:GLU:HG3	1:169:A:LYS:HE3	5	0.13
(1,42)	1:37:A:SER:HA	1:39:A:ASP:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:41:A:LYS:HE2	1:120:A:GLU:HB2	7	0.13
(1,23)	1:41:A:LYS:HE2	1:120:A:GLU:HB3	7	0.13
(1,23)	1:41:A:LYS:HE3	1:120:A:GLU:HB2	7	0.13
(1,23)	1:41:A:LYS:HE3	1:120:A:GLU:HB3	7	0.13
(1,1679)	1:162:A:GLN:HE21	1:165:A:VAL:HG11	7	0.12
(1,1679)	1:162:A:GLN:HE21	1:165:A:VAL:HG12	7	0.12
(1,1679)	1:162:A:GLN:HE21	1:165:A:VAL:HG13	7	0.12
(1,1679)	1:162:A:GLN:HE21	1:165:A:VAL:HG21	7	0.12
(1,1679)	1:162:A:GLN:HE21	1:165:A:VAL:HG22	7	0.12
(1,1679)	1:162:A:GLN:HE21	1:165:A:VAL:HG23	7	0.12
(1,1679)	1:162:A:GLN:HE22	1:165:A:VAL:HG11	7	0.12
(1,1679)	1:162:A:GLN:HE22	1:165:A:VAL:HG12	7	0.12
(1,1679)	1:162:A:GLN:HE22	1:165:A:VAL:HG13	7	0.12
(1,1679)	1:162:A:GLN:HE22	1:165:A:VAL:HG21	7	0.12
(1,1679)	1:162:A:GLN:HE22	1:165:A:VAL:HG22	7	0.12
(1,1679)	1:162:A:GLN:HE22	1:165:A:VAL:HG23	7	0.12
(1,1665)	1:158:A:GLN:HG2	1:161:A:ASN:H	5	0.12
(1,1665)	1:158:A:GLN:HG3	1:161:A:ASN:H	5	0.12
(1,1628)	1:141:A:SER:HB2	1:146:A:ILE:HD11	3	0.12
(1,1628)	1:141:A:SER:HB2	1:146:A:ILE:HD12	3	0.12
(1,1628)	1:141:A:SER:HB2	1:146:A:ILE:HD13	3	0.12
(1,1628)	1:141:A:SER:HB3	1:146:A:ILE:HD11	3	0.12
(1,1628)	1:141:A:SER:HB3	1:146:A:ILE:HD12	3	0.12
(1,1628)	1:141:A:SER:HB3	1:146:A:ILE:HD13	3	0.12
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG2	7	0.12
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG3	7	0.12
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG2	7	0.12
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG3	7	0.12
(1,1615)	1:137:A:VAL:HG11	1:138:A:LEU:HD11	9	0.12
(1,1615)	1:137:A:VAL:HG11	1:138:A:LEU:HD12	9	0.12
(1,1615)	1:137:A:VAL:HG11	1:138:A:LEU:HD13	9	0.12
(1,1615)	1:137:A:VAL:HG11	1:138:A:LEU:HD21	9	0.12
(1,1615)	1:137:A:VAL:HG11	1:138:A:LEU:HD22	9	0.12
(1,1615)	1:137:A:VAL:HG11	1:138:A:LEU:HD23	9	0.12
(1,1615)	1:137:A:VAL:HG12	1:138:A:LEU:HD11	9	0.12
(1,1615)	1:137:A:VAL:HG12	1:138:A:LEU:HD12	9	0.12
(1,1615)	1:137:A:VAL:HG12	1:138:A:LEU:HD13	9	0.12
(1,1615)	1:137:A:VAL:HG12	1:138:A:LEU:HD21	9	0.12
(1,1615)	1:137:A:VAL:HG12	1:138:A:LEU:HD22	9	0.12
(1,1615)	1:137:A:VAL:HG12	1:138:A:LEU:HD23	9	0.12
(1,1615)	1:137:A:VAL:HG13	1:138:A:LEU:HD11	9	0.12
(1,1615)	1:137:A:VAL:HG13	1:138:A:LEU:HD12	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1615)	1:137:A:VAL:HG13	1:138:A:LEU:HD13	9	0.12
(1,1615)	1:137:A:VAL:HG13	1:138:A:LEU:HD21	9	0.12
(1,1615)	1:137:A:VAL:HG13	1:138:A:LEU:HD22	9	0.12
(1,1615)	1:137:A:VAL:HG13	1:138:A:LEU:HD23	9	0.12
(1,1615)	1:137:A:VAL:HG21	1:138:A:LEU:HD11	9	0.12
(1,1615)	1:137:A:VAL:HG21	1:138:A:LEU:HD12	9	0.12
(1,1615)	1:137:A:VAL:HG21	1:138:A:LEU:HD13	9	0.12
(1,1615)	1:137:A:VAL:HG21	1:138:A:LEU:HD21	9	0.12
(1,1615)	1:137:A:VAL:HG21	1:138:A:LEU:HD22	9	0.12
(1,1615)	1:137:A:VAL:HG21	1:138:A:LEU:HD23	9	0.12
(1,1615)	1:137:A:VAL:HG22	1:138:A:LEU:HD11	9	0.12
(1,1615)	1:137:A:VAL:HG22	1:138:A:LEU:HD12	9	0.12
(1,1615)	1:137:A:VAL:HG22	1:138:A:LEU:HD13	9	0.12
(1,1615)	1:137:A:VAL:HG22	1:138:A:LEU:HD21	9	0.12
(1,1615)	1:137:A:VAL:HG22	1:138:A:LEU:HD22	9	0.12
(1,1615)	1:137:A:VAL:HG22	1:138:A:LEU:HD23	9	0.12
(1,1615)	1:137:A:VAL:HG23	1:138:A:LEU:HD11	9	0.12
(1,1615)	1:137:A:VAL:HG23	1:138:A:LEU:HD12	9	0.12
(1,1615)	1:137:A:VAL:HG23	1:138:A:LEU:HD13	9	0.12
(1,1615)	1:137:A:VAL:HG23	1:138:A:LEU:HD21	9	0.12
(1,1615)	1:137:A:VAL:HG23	1:138:A:LEU:HD22	9	0.12
(1,1615)	1:137:A:VAL:HG23	1:138:A:LEU:HD23	9	0.12
(1,1603)	1:134:A:LYS:HE2	1:138:A:LEU:HD11	9	0.12
(1,1603)	1:134:A:LYS:HE2	1:138:A:LEU:HD12	9	0.12
(1,1603)	1:134:A:LYS:HE2	1:138:A:LEU:HD13	9	0.12
(1,1603)	1:134:A:LYS:HE2	1:138:A:LEU:HD21	9	0.12
(1,1603)	1:134:A:LYS:HE2	1:138:A:LEU:HD22	9	0.12
(1,1603)	1:134:A:LYS:HE2	1:138:A:LEU:HD23	9	0.12
(1,1603)	1:134:A:LYS:HE3	1:138:A:LEU:HD11	9	0.12
(1,1603)	1:134:A:LYS:HE3	1:138:A:LEU:HD12	9	0.12
(1,1603)	1:134:A:LYS:HE3	1:138:A:LEU:HD13	9	0.12
(1,1603)	1:134:A:LYS:HE3	1:138:A:LEU:HD21	9	0.12
(1,1603)	1:134:A:LYS:HE3	1:138:A:LEU:HD22	9	0.12
(1,1603)	1:134:A:LYS:HE3	1:138:A:LEU:HD23	9	0.12
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA2	9	0.12
(1,1575)	1:131:A:ILE:HB	1:132:A:GLY:HA3	9	0.12
(1,1562)	1:122:A:VAL:HG11	1:134:A:LYS:HB2	4	0.12
(1,1562)	1:122:A:VAL:HG11	1:134:A:LYS:HB3	4	0.12
(1,1562)	1:122:A:VAL:HG12	1:134:A:LYS:HB2	4	0.12
(1,1562)	1:122:A:VAL:HG12	1:134:A:LYS:HB3	4	0.12
(1,1562)	1:122:A:VAL:HG13	1:134:A:LYS:HB2	4	0.12
(1,1562)	1:122:A:VAL:HG13	1:134:A:LYS:HB3	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1562)	1:122:A:VAL:HG21	1:134:A:LYS:HB2	4	0.12
(1,1562)	1:122:A:VAL:HG21	1:134:A:LYS:HB3	4	0.12
(1,1562)	1:122:A:VAL:HG22	1:134:A:LYS:HB2	4	0.12
(1,1562)	1:122:A:VAL:HG22	1:134:A:LYS:HB3	4	0.12
(1,1562)	1:122:A:VAL:HG23	1:134:A:LYS:HB2	4	0.12
(1,1562)	1:122:A:VAL:HG23	1:134:A:LYS:HB3	4	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD11	4	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD12	4	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD13	4	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD21	4	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD22	4	0.12
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD23	4	0.12
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD11	1	0.12
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD12	1	0.12
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD13	1	0.12
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD21	1	0.12
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD22	1	0.12
(1,1463)	1:96:A:GLU:HG2	1:153:A:LEU:HD23	1	0.12
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD11	1	0.12
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD12	1	0.12
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD13	1	0.12
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD21	1	0.12
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD22	1	0.12
(1,1463)	1:96:A:GLU:HG3	1:153:A:LEU:HD23	1	0.12
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB2	4	0.12
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB3	4	0.12
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB2	4	0.12
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB3	4	0.12
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB2	4	0.12
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB3	4	0.12
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB2	4	0.12
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB3	4	0.12
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB2	4	0.12
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB3	4	0.12
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB2	4	0.12
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB3	4	0.12
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB2	5	0.12
(1,1457)	1:92:A:LEU:HD11	1:160:A:GLU:HB3	5	0.12
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB2	5	0.12
(1,1457)	1:92:A:LEU:HD12	1:160:A:GLU:HB3	5	0.12
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB2	5	0.12
(1,1457)	1:92:A:LEU:HD13	1:160:A:GLU:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB2	5	0.12
(1,1457)	1:92:A:LEU:HD21	1:160:A:GLU:HB3	5	0.12
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB2	5	0.12
(1,1457)	1:92:A:LEU:HD22	1:160:A:GLU:HB3	5	0.12
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB2	5	0.12
(1,1457)	1:92:A:LEU:HD23	1:160:A:GLU:HB3	5	0.12
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG2	8	0.12
(1,1387)	1:64:A:LEU:HD11	1:69:A:LYS:HG3	8	0.12
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG2	8	0.12
(1,1387)	1:64:A:LEU:HD12	1:69:A:LYS:HG3	8	0.12
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG2	8	0.12
(1,1387)	1:64:A:LEU:HD13	1:69:A:LYS:HG3	8	0.12
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG2	8	0.12
(1,1387)	1:64:A:LEU:HD21	1:69:A:LYS:HG3	8	0.12
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG2	8	0.12
(1,1387)	1:64:A:LEU:HD22	1:69:A:LYS:HG3	8	0.12
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG2	8	0.12
(1,1387)	1:64:A:LEU:HD23	1:69:A:LYS:HG3	8	0.12
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG21	5	0.12
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG22	5	0.12
(1,1381)	1:61:A:PHE:HB2	1:66:A:THR:HG23	5	0.12
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG21	5	0.12
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG22	5	0.12
(1,1381)	1:61:A:PHE:HB3	1:66:A:THR:HG23	5	0.12
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD11	2	0.12
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD12	2	0.12
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD13	2	0.12
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD21	2	0.12
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD22	2	0.12
(1,1380)	1:61:A:PHE:HB2	1:64:A:LEU:HD23	2	0.12
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD11	2	0.12
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD12	2	0.12
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD13	2	0.12
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD21	2	0.12
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD22	2	0.12
(1,1380)	1:61:A:PHE:HB3	1:64:A:LEU:HD23	2	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD11	8	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD12	8	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD13	8	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD21	8	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD22	8	0.12
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD23	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB2	1	0.12
(1,1373)	1:60:A:ALA:H	1:64:A:LEU:HB3	1	0.12
(1,1361)	1:56:A:VAL:HG11	1:76:A:ALA:HB1	7	0.12
(1,1361)	1:56:A:VAL:HG11	1:76:A:ALA:HB2	7	0.12
(1,1361)	1:56:A:VAL:HG11	1:76:A:ALA:HB3	7	0.12
(1,1361)	1:56:A:VAL:HG12	1:76:A:ALA:HB1	7	0.12
(1,1361)	1:56:A:VAL:HG12	1:76:A:ALA:HB2	7	0.12
(1,1361)	1:56:A:VAL:HG12	1:76:A:ALA:HB3	7	0.12
(1,1361)	1:56:A:VAL:HG13	1:76:A:ALA:HB1	7	0.12
(1,1361)	1:56:A:VAL:HG13	1:76:A:ALA:HB2	7	0.12
(1,1361)	1:56:A:VAL:HG13	1:76:A:ALA:HB3	7	0.12
(1,1361)	1:56:A:VAL:HG21	1:76:A:ALA:HB1	7	0.12
(1,1361)	1:56:A:VAL:HG21	1:76:A:ALA:HB2	7	0.12
(1,1361)	1:56:A:VAL:HG21	1:76:A:ALA:HB3	7	0.12
(1,1361)	1:56:A:VAL:HG22	1:76:A:ALA:HB1	7	0.12
(1,1361)	1:56:A:VAL:HG22	1:76:A:ALA:HB2	7	0.12
(1,1361)	1:56:A:VAL:HG22	1:76:A:ALA:HB3	7	0.12
(1,1361)	1:56:A:VAL:HG23	1:76:A:ALA:HB1	7	0.12
(1,1361)	1:56:A:VAL:HG23	1:76:A:ALA:HB2	7	0.12
(1,1361)	1:56:A:VAL:HG23	1:76:A:ALA:HB3	7	0.12
(1,1359)	1:56:A:VAL:HG11	1:58:A:PHE:HA	8	0.12
(1,1359)	1:56:A:VAL:HG12	1:58:A:PHE:HA	8	0.12
(1,1359)	1:56:A:VAL:HG13	1:58:A:PHE:HA	8	0.12
(1,1359)	1:56:A:VAL:HG21	1:58:A:PHE:HA	8	0.12
(1,1359)	1:56:A:VAL:HG22	1:58:A:PHE:HA	8	0.12
(1,1359)	1:56:A:VAL:HG23	1:58:A:PHE:HA	8	0.12
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG2	1	0.12
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG3	1	0.12
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG2	1	0.12
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG3	1	0.12
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG2	1	0.12
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG3	1	0.12
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG2	1	0.12
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG3	1	0.12
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG2	1	0.12
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG3	1	0.12
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG2	1	0.12
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG3	1	0.12
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG2	6	0.12
(1,1340)	1:45:A:LEU:HD11	1:46:A:LYS:HG3	6	0.12
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG2	6	0.12
(1,1340)	1:45:A:LEU:HD12	1:46:A:LYS:HG3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG2	6	0.12
(1,1340)	1:45:A:LEU:HD13	1:46:A:LYS:HG3	6	0.12
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG2	6	0.12
(1,1340)	1:45:A:LEU:HD21	1:46:A:LYS:HG3	6	0.12
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG2	6	0.12
(1,1340)	1:45:A:LEU:HD22	1:46:A:LYS:HG3	6	0.12
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG2	6	0.12
(1,1340)	1:45:A:LEU:HD23	1:46:A:LYS:HG3	6	0.12
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG21	10	0.12
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG22	10	0.12
(1,1281)	1:37:A:SER:HB2	1:95:A:ILE:HG23	10	0.12
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG21	10	0.12
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG22	10	0.12
(1,1281)	1:37:A:SER:HB3	1:95:A:ILE:HG23	10	0.12
(1,1265)	1:33:A:LEU:HD11	1:94:A:ILE:HD11	9	0.12
(1,1265)	1:33:A:LEU:HD11	1:94:A:ILE:HD12	9	0.12
(1,1265)	1:33:A:LEU:HD11	1:94:A:ILE:HD13	9	0.12
(1,1265)	1:33:A:LEU:HD12	1:94:A:ILE:HD11	9	0.12
(1,1265)	1:33:A:LEU:HD12	1:94:A:ILE:HD12	9	0.12
(1,1265)	1:33:A:LEU:HD12	1:94:A:ILE:HD13	9	0.12
(1,1265)	1:33:A:LEU:HD13	1:94:A:ILE:HD11	9	0.12
(1,1265)	1:33:A:LEU:HD13	1:94:A:ILE:HD12	9	0.12
(1,1265)	1:33:A:LEU:HD13	1:94:A:ILE:HD13	9	0.12
(1,1265)	1:33:A:LEU:HD21	1:94:A:ILE:HD11	9	0.12
(1,1265)	1:33:A:LEU:HD21	1:94:A:ILE:HD12	9	0.12
(1,1265)	1:33:A:LEU:HD21	1:94:A:ILE:HD13	9	0.12
(1,1265)	1:33:A:LEU:HD22	1:94:A:ILE:HD11	9	0.12
(1,1265)	1:33:A:LEU:HD22	1:94:A:ILE:HD12	9	0.12
(1,1265)	1:33:A:LEU:HD22	1:94:A:ILE:HD13	9	0.12
(1,1265)	1:33:A:LEU:HD23	1:94:A:ILE:HD11	9	0.12
(1,1265)	1:33:A:LEU:HD23	1:94:A:ILE:HD12	9	0.12
(1,1265)	1:33:A:LEU:HD23	1:94:A:ILE:HD13	9	0.12
(1,1258)	1:33:A:LEU:HB2	1:95:A:ILE:HG21	8	0.12
(1,1258)	1:33:A:LEU:HB2	1:95:A:ILE:HG22	8	0.12
(1,1258)	1:33:A:LEU:HB2	1:95:A:ILE:HG23	8	0.12
(1,1258)	1:33:A:LEU:HB3	1:95:A:ILE:HG21	8	0.12
(1,1258)	1:33:A:LEU:HB3	1:95:A:ILE:HG22	8	0.12
(1,1258)	1:33:A:LEU:HB3	1:95:A:ILE:HG23	8	0.12
(1,1228)	1:86:A:VAL:H	1:167:A:LYS:HB2	8	0.12
(1,1228)	1:86:A:VAL:H	1:167:A:LYS:HB3	8	0.12
(1,1182)	1:55:A:GLY:H	1:56:A:VAL:HB	9	0.12
(1,1154)	1:42:A:ASN:HD22	1:43:A:LYS:HD2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:42:A:ASN:HD22	1:43:A:LYS:HD3	1	0.12
(1,1117)	1:101:A:LYS:HG2	1:104:A:GLU:H	6	0.12
(1,1117)	1:101:A:LYS:HG3	1:104:A:GLU:H	6	0.12
(1,941)	1:156:A:LYS:HG2	1:160:A:GLU:H	5	0.12
(1,941)	1:156:A:LYS:HG3	1:160:A:GLU:H	5	0.12
(1,794)	1:52:A:THR:HG21	1:58:A:PHE:HD1	3	0.12
(1,794)	1:52:A:THR:HG21	1:58:A:PHE:HD2	3	0.12
(1,794)	1:52:A:THR:HG22	1:58:A:PHE:HD1	3	0.12
(1,794)	1:52:A:THR:HG22	1:58:A:PHE:HD2	3	0.12
(1,794)	1:52:A:THR:HG23	1:58:A:PHE:HD1	3	0.12
(1,794)	1:52:A:THR:HG23	1:58:A:PHE:HD2	3	0.12
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	8	0.12
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	8	0.12
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	8	0.12
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	8	0.12
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	8	0.12
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	8	0.12
(1,748)	1:39:A:ASP:HA	1:42:A:ASN:HD22	1	0.12
(1,712)	1:41:A:LYS:H	1:41:A:LYS:HD2	8	0.12
(1,712)	1:41:A:LYS:H	1:41:A:LYS:HD3	8	0.12
(1,699)	1:45:A:LEU:HG	1:46:A:LYS:HA	9	0.12
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG2	7	0.12
(1,684)	1:144:A:ASN:HA	1:145:A:PRO:HG3	7	0.12
(1,679)	1:29:A:THR:HA	1:30:A:ASN:HA	6	0.12
(1,665)	1:51:A:ALA:HA	1:77:A:LEU:HA	1	0.12
(1,662)	1:146:A:ILE:HD11	1:155:A:ALA:H	1	0.12
(1,662)	1:146:A:ILE:HD12	1:155:A:ALA:H	1	0.12
(1,662)	1:146:A:ILE:HD13	1:155:A:ALA:H	1	0.12
(1,660)	1:146:A:ILE:H	1:146:A:ILE:HD11	7	0.12
(1,660)	1:146:A:ILE:H	1:146:A:ILE:HD12	7	0.12
(1,660)	1:146:A:ILE:H	1:146:A:ILE:HD13	7	0.12
(1,642)	1:38:A:LYS:HB2	1:39:A:ASP:HA	2	0.12
(1,642)	1:38:A:LYS:HB3	1:39:A:ASP:HA	2	0.12
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD11	9	0.12
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD12	9	0.12
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD13	9	0.12
(1,593)	1:131:A:ILE:H	1:131:A:ILE:HD11	5	0.12
(1,593)	1:131:A:ILE:H	1:131:A:ILE:HD12	5	0.12
(1,593)	1:131:A:ILE:H	1:131:A:ILE:HD13	5	0.12
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD11	8	0.12
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD12	8	0.12
(1,565)	1:118:A:MET:HA	1:159:A:ILE:HD13	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:99:A:ALA:HB1	1:149:A:ALA:HB1	4	0.12
(1,489)	1:99:A:ALA:HB1	1:149:A:ALA:HB2	4	0.12
(1,489)	1:99:A:ALA:HB1	1:149:A:ALA:HB3	4	0.12
(1,489)	1:99:A:ALA:HB2	1:149:A:ALA:HB1	4	0.12
(1,489)	1:99:A:ALA:HB2	1:149:A:ALA:HB2	4	0.12
(1,489)	1:99:A:ALA:HB2	1:149:A:ALA:HB3	4	0.12
(1,489)	1:99:A:ALA:HB3	1:149:A:ALA:HB1	4	0.12
(1,489)	1:99:A:ALA:HB3	1:149:A:ALA:HB2	4	0.12
(1,489)	1:99:A:ALA:HB3	1:149:A:ALA:HB3	4	0.12
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	4	0.12
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	4	0.12
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	4	0.12
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	4	0.12
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	4	0.12
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	4	0.12
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	4	0.12
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	4	0.12
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	4	0.12
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB1	7	0.12
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB2	7	0.12
(1,473)	1:114:A:MET:HE1	1:155:A:ALA:HB3	7	0.12
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB1	7	0.12
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB2	7	0.12
(1,473)	1:114:A:MET:HE2	1:155:A:ALA:HB3	7	0.12
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB1	7	0.12
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB2	7	0.12
(1,473)	1:114:A:MET:HE3	1:155:A:ALA:HB3	7	0.12
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	3	0.12
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	3	0.12
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	3	0.12
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB1	9	0.12
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB2	9	0.12
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB3	9	0.12
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE1	5	0.12
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE2	5	0.12
(1,425)	1:98:A:GLU:H	1:118:A:MET:HE3	5	0.12
(1,414)	1:84:A:ALA:HB1	1:128:A:VAL:HG21	8	0.12
(1,414)	1:84:A:ALA:HB1	1:128:A:VAL:HG22	8	0.12
(1,414)	1:84:A:ALA:HB1	1:128:A:VAL:HG23	8	0.12
(1,414)	1:84:A:ALA:HB2	1:128:A:VAL:HG21	8	0.12
(1,414)	1:84:A:ALA:HB2	1:128:A:VAL:HG22	8	0.12
(1,414)	1:84:A:ALA:HB2	1:128:A:VAL:HG23	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:84:A:ALA:HB3	1:128:A:VAL:HG21	8	0.12
(1,414)	1:84:A:ALA:HB3	1:128:A:VAL:HG22	8	0.12
(1,414)	1:84:A:ALA:HB3	1:128:A:VAL:HG23	8	0.12
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	1	0.12
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	1	0.12
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	1	0.12
(1,390)	1:82:A:VAL:HG11	1:170:A:GLN:HG3	3	0.12
(1,390)	1:82:A:VAL:HG12	1:170:A:GLN:HG3	3	0.12
(1,390)	1:82:A:VAL:HG13	1:170:A:GLN:HG3	3	0.12
(1,318)	1:102:A:LEU:HD11	1:106:A:GLY:H	8	0.12
(1,318)	1:102:A:LEU:HD12	1:106:A:GLY:H	8	0.12
(1,318)	1:102:A:LEU:HD13	1:106:A:GLY:H	8	0.12
(1,286)	1:40:A:LEU:HD11	1:43:A:LYS:H	2	0.12
(1,286)	1:40:A:LEU:HD12	1:43:A:LYS:H	2	0.12
(1,286)	1:40:A:LEU:HD13	1:43:A:LYS:H	2	0.12
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD11	7	0.12
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD12	7	0.12
(1,262)	1:45:A:LEU:HA	1:45:A:LEU:HD13	7	0.12
(1,231)	1:48:A:LYS:HG2	1:49:A:LYS:H	6	0.12
(1,231)	1:48:A:LYS:HG3	1:49:A:LYS:H	6	0.12
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG2	6	0.12
(1,222)	1:102:A:LEU:HG	1:110:A:GLN:HG3	6	0.12
(1,154)	1:81:A:LYS:HD2	1:128:A:VAL:HB	6	0.12
(1,154)	1:81:A:LYS:HD3	1:128:A:VAL:HB	6	0.12
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	4	0.12
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	4	0.12
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	4	0.12
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	4	0.12
(1,103)	1:158:A:GLN:H	1:158:A:GLN:HG3	3	0.12
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD2	3	0.12
(1,8)	1:136:A:ARG:H	1:136:A:ARG:HD3	3	0.12
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG2	4	0.11
(1,1660)	1:157:A:ALA:HB1	1:160:A:GLU:HG3	4	0.11
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG2	4	0.11
(1,1660)	1:157:A:ALA:HB2	1:160:A:GLU:HG3	4	0.11
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG2	4	0.11
(1,1660)	1:157:A:ALA:HB3	1:160:A:GLU:HG3	4	0.11
(1,1658)	1:155:A:ALA:HA	1:158:A:GLN:HG2	3	0.11
(1,1658)	1:155:A:ALA:HA	1:158:A:GLN:HG3	3	0.11
(1,1633)	1:144:A:ASN:HD21	1:145:A:PRO:HG2	5	0.11
(1,1633)	1:144:A:ASN:HD21	1:145:A:PRO:HG3	5	0.11
(1,1633)	1:144:A:ASN:HD22	1:145:A:PRO:HG2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1633)	1:144:A:ASN:HD22	1:145:A:PRO:HG3	5	0.11
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG2	4	0.11
(1,1624)	1:139:A:GLU:HB2	1:142:A:LYS:HG3	4	0.11
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG2	4	0.11
(1,1624)	1:139:A:GLU:HB3	1:142:A:LYS:HG3	4	0.11
(1,1591)	1:133:A:LEU:HD11	1:163:A:LEU:HA	2	0.11
(1,1591)	1:133:A:LEU:HD12	1:163:A:LEU:HA	2	0.11
(1,1591)	1:133:A:LEU:HD13	1:163:A:LEU:HA	2	0.11
(1,1591)	1:133:A:LEU:HD21	1:163:A:LEU:HA	2	0.11
(1,1591)	1:133:A:LEU:HD22	1:163:A:LEU:HA	2	0.11
(1,1591)	1:133:A:LEU:HD23	1:163:A:LEU:HA	2	0.11
(1,1539)	1:118:A:MET:HB2	1:119:A:LEU:HD11	9	0.11
(1,1539)	1:118:A:MET:HB2	1:119:A:LEU:HD12	9	0.11
(1,1539)	1:118:A:MET:HB2	1:119:A:LEU:HD13	9	0.11
(1,1539)	1:118:A:MET:HB2	1:119:A:LEU:HD21	9	0.11
(1,1539)	1:118:A:MET:HB2	1:119:A:LEU:HD22	9	0.11
(1,1539)	1:118:A:MET:HB2	1:119:A:LEU:HD23	9	0.11
(1,1511)	1:112:A:LEU:HB2	1:116:A:ASP:H	6	0.11
(1,1511)	1:112:A:LEU:HB3	1:116:A:ASP:H	6	0.11
(1,1490)	1:102:A:LEU:HD11	1:110:A:GLN:HE21	3	0.11
(1,1490)	1:102:A:LEU:HD11	1:110:A:GLN:HE22	3	0.11
(1,1490)	1:102:A:LEU:HD12	1:110:A:GLN:HE21	3	0.11
(1,1490)	1:102:A:LEU:HD12	1:110:A:GLN:HE22	3	0.11
(1,1490)	1:102:A:LEU:HD13	1:110:A:GLN:HE21	3	0.11
(1,1490)	1:102:A:LEU:HD13	1:110:A:GLN:HE22	3	0.11
(1,1490)	1:102:A:LEU:HD21	1:110:A:GLN:HE21	3	0.11
(1,1490)	1:102:A:LEU:HD21	1:110:A:GLN:HE22	3	0.11
(1,1490)	1:102:A:LEU:HD22	1:110:A:GLN:HE21	3	0.11
(1,1490)	1:102:A:LEU:HD22	1:110:A:GLN:HE22	3	0.11
(1,1490)	1:102:A:LEU:HD23	1:110:A:GLN:HE21	3	0.11
(1,1490)	1:102:A:LEU:HD23	1:110:A:GLN:HE22	3	0.11
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD11	10	0.11
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD12	10	0.11
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD13	10	0.11
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD21	10	0.11
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD22	10	0.11
(1,1474)	1:100:A:LEU:HA	1:100:A:LEU:HD23	10	0.11
(1,1437)	1:86:A:VAL:HG11	1:167:A:LYS:HD2	7	0.11
(1,1437)	1:86:A:VAL:HG11	1:167:A:LYS:HD3	7	0.11
(1,1437)	1:86:A:VAL:HG12	1:167:A:LYS:HD2	7	0.11
(1,1437)	1:86:A:VAL:HG12	1:167:A:LYS:HD3	7	0.11
(1,1437)	1:86:A:VAL:HG13	1:167:A:LYS:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:86:A:VAL:HG13	1:167:A:LYS:HD3	7	0.11
(1,1437)	1:86:A:VAL:HG21	1:167:A:LYS:HD2	7	0.11
(1,1437)	1:86:A:VAL:HG21	1:167:A:LYS:HD3	7	0.11
(1,1437)	1:86:A:VAL:HG22	1:167:A:LYS:HD2	7	0.11
(1,1437)	1:86:A:VAL:HG22	1:167:A:LYS:HD3	7	0.11
(1,1437)	1:86:A:VAL:HG23	1:167:A:LYS:HD2	7	0.11
(1,1437)	1:86:A:VAL:HG23	1:167:A:LYS:HD3	7	0.11
(1,1426)	1:83:A:GLN:HE21	1:87:A:GLU:HG2	10	0.11
(1,1426)	1:83:A:GLN:HE21	1:87:A:GLU:HG3	10	0.11
(1,1426)	1:83:A:GLN:HE22	1:87:A:GLU:HG2	10	0.11
(1,1426)	1:83:A:GLN:HE22	1:87:A:GLU:HG3	10	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG11	6	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG12	6	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG13	6	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG21	6	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG22	6	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG23	6	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG11	6	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG12	6	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG13	6	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG21	6	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG22	6	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG23	6	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG11	10	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG12	10	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG13	10	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG21	10	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG22	10	0.11
(1,1393)	1:69:A:LYS:HE2	1:70:A:VAL:HG23	10	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG11	10	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG12	10	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG13	10	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG21	10	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG22	10	0.11
(1,1393)	1:69:A:LYS:HE3	1:70:A:VAL:HG23	10	0.11
(1,1376)	1:60:A:ALA:HA	1:64:A:LEU:HB2	4	0.11
(1,1376)	1:60:A:ALA:HA	1:64:A:LEU:HB3	4	0.11
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD1	9	0.11
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD2	9	0.11
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD1	9	0.11
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD2	9	0.11
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD1	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD2	9	0.11
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD1	9	0.11
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD2	9	0.11
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD1	9	0.11
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD2	9	0.11
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD1	9	0.11
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD2	9	0.11
(1,1344)	1:47:A:ILE:HD11	1:83:A:GLN:HG2	7	0.11
(1,1344)	1:47:A:ILE:HD11	1:83:A:GLN:HG3	7	0.11
(1,1344)	1:47:A:ILE:HD12	1:83:A:GLN:HG2	7	0.11
(1,1344)	1:47:A:ILE:HD12	1:83:A:GLN:HG3	7	0.11
(1,1344)	1:47:A:ILE:HD13	1:83:A:GLN:HG2	7	0.11
(1,1344)	1:47:A:ILE:HD13	1:83:A:GLN:HG3	7	0.11
(1,1314)	1:41:A:LYS:H	1:121:A:VAL:HG11	9	0.11
(1,1314)	1:41:A:LYS:H	1:121:A:VAL:HG12	9	0.11
(1,1314)	1:41:A:LYS:H	1:121:A:VAL:HG13	9	0.11
(1,1314)	1:41:A:LYS:H	1:121:A:VAL:HG21	9	0.11
(1,1314)	1:41:A:LYS:H	1:121:A:VAL:HG22	9	0.11
(1,1314)	1:41:A:LYS:H	1:121:A:VAL:HG23	9	0.11
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB2	4	0.11
(1,1279)	1:37:A:SER:HB2	1:38:A:LYS:HB3	4	0.11
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB2	4	0.11
(1,1279)	1:37:A:SER:HB3	1:38:A:LYS:HB3	4	0.11
(1,1195)	1:111:A:PHE:H	1:147:A:ASN:HA	2	0.11
(1,1181)	1:52:A:THR:HG21	1:55:A:GLY:H	10	0.11
(1,1181)	1:52:A:THR:HG22	1:55:A:GLY:H	10	0.11
(1,1181)	1:52:A:THR:HG23	1:55:A:GLY:H	10	0.11
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD11	2	0.11
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD12	2	0.11
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD13	2	0.11
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD11	8	0.11
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD12	8	0.11
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD13	8	0.11
(1,1166)	1:133:A:LEU:HD11	1:162:A:GLN:HE22	3	0.11
(1,1166)	1:133:A:LEU:HD12	1:162:A:GLN:HE22	3	0.11
(1,1166)	1:133:A:LEU:HD13	1:162:A:GLN:HE22	3	0.11
(1,1156)	1:62:A:THR:H	1:66:A:THR:HG21	2	0.11
(1,1156)	1:62:A:THR:H	1:66:A:THR:HG22	2	0.11
(1,1156)	1:62:A:THR:H	1:66:A:THR:HG23	2	0.11
(1,1129)	1:101:A:LYS:HD2	1:102:A:LEU:H	7	0.11
(1,1129)	1:101:A:LYS:HD3	1:102:A:LEU:H	7	0.11
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:96:A:GLU:H	1:156:A:LYS:HG3	5	0.11
(1,1042)	1:121:A:VAL:HB	1:124:A:SER:H	3	0.11
(1,1042)	1:121:A:VAL:HB	1:124:A:SER:H	5	0.11
(1,925)	1:40:A:LEU:H	1:121:A:VAL:HA	7	0.11
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD1	2	0.11
(1,913)	1:90:A:LYS:H	1:91:A:PHE:HD2	2	0.11
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE1	2	0.11
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE2	2	0.11
(1,785)	1:111:A:PHE:HD1	1:114:A:MET:HE3	2	0.11
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE1	2	0.11
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE2	2	0.11
(1,785)	1:111:A:PHE:HD2	1:114:A:MET:HE3	2	0.11
(1,755)	1:44:A:ILE:HD11	1:124:A:SER:H	5	0.11
(1,755)	1:44:A:ILE:HD12	1:124:A:SER:H	5	0.11
(1,755)	1:44:A:ILE:HD13	1:124:A:SER:H	5	0.11
(1,686)	1:26:A:VAL:HA	1:27:A:GLU:H	9	0.11
(1,632)	1:44:A:ILE:HD11	1:125:A:LEU:HA	1	0.11
(1,632)	1:44:A:ILE:HD12	1:125:A:LEU:HA	1	0.11
(1,632)	1:44:A:ILE:HD13	1:125:A:LEU:HA	1	0.11
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	1	0.11
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD11	4	0.11
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD12	4	0.11
(1,602)	1:137:A:VAL:HA	1:159:A:ILE:HD13	4	0.11
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD11	10	0.11
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD12	10	0.11
(1,601)	1:172:A:ILE:HA	1:172:A:ILE:HD13	10	0.11
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB1	1	0.11
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB2	1	0.11
(1,585)	1:47:A:ILE:HD11	1:84:A:ALA:HB3	1	0.11
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB1	1	0.11
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB2	1	0.11
(1,585)	1:47:A:ILE:HD12	1:84:A:ALA:HB3	1	0.11
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB1	1	0.11
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB2	1	0.11
(1,585)	1:47:A:ILE:HD13	1:84:A:ALA:HB3	1	0.11
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD11	9	0.11
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD12	9	0.11
(1,558)	1:126:A:GLU:H	1:130:A:ILE:HD13	9	0.11
(1,528)	1:114:A:MET:HE1	1:118:A:MET:HG2	2	0.11
(1,528)	1:114:A:MET:HE1	1:118:A:MET:HG3	2	0.11
(1,528)	1:114:A:MET:HE2	1:118:A:MET:HG2	2	0.11
(1,528)	1:114:A:MET:HE2	1:118:A:MET:HG3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,528)	1:114:A:MET:HE3	1:118:A:MET:HG2	2	0.11
(1,528)	1:114:A:MET:HE3	1:118:A:MET:HG3	2	0.11
(1,478)	1:99:A:ALA:HB1	1:153:A:LEU:HG	5	0.11
(1,478)	1:99:A:ALA:HB2	1:153:A:LEU:HG	5	0.11
(1,478)	1:99:A:ALA:HB3	1:153:A:LEU:HG	5	0.11
(1,478)	1:99:A:ALA:HB1	1:153:A:LEU:HG	9	0.11
(1,478)	1:99:A:ALA:HB2	1:153:A:LEU:HG	9	0.11
(1,478)	1:99:A:ALA:HB3	1:153:A:LEU:HG	9	0.11
(1,462)	1:108:A:SER:HB2	1:147:A:ASN:HB2	4	0.11
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB1	10	0.11
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB2	10	0.11
(1,451)	1:30:A:ASN:HA	1:31:A:ALA:HB3	10	0.11
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG21	5	0.11
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG22	5	0.11
(1,416)	1:44:A:ILE:HA	1:47:A:ILE:HG23	5	0.11
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG21	9	0.11
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG22	9	0.11
(1,395)	1:85:A:ILE:HB	1:88:A:THR:HG23	9	0.11
(1,302)	1:150:A:GLU:HA	1:153:A:LEU:HD21	8	0.11
(1,302)	1:150:A:GLU:HA	1:153:A:LEU:HD22	8	0.11
(1,302)	1:150:A:GLU:HA	1:153:A:LEU:HD23	8	0.11
(1,225)	1:77:A:LEU:HG	1:81:A:LYS:HG2	7	0.11
(1,225)	1:77:A:LEU:HG	1:81:A:LYS:HG3	7	0.11
(1,225)	1:77:A:LEU:HG	1:81:A:LYS:HG2	8	0.11
(1,225)	1:77:A:LEU:HG	1:81:A:LYS:HG3	8	0.11
(1,218)	1:109:A:GLY:HA2	1:112:A:LEU:HG	3	0.11
(1,218)	1:109:A:GLY:HA3	1:112:A:LEU:HG	3	0.11
(1,181)	1:41:A:LYS:HD2	1:120:A:GLU:HB2	6	0.11
(1,181)	1:41:A:LYS:HD2	1:120:A:GLU:HB3	6	0.11
(1,181)	1:41:A:LYS:HD3	1:120:A:GLU:HB2	6	0.11
(1,181)	1:41:A:LYS:HD3	1:120:A:GLU:HB3	6	0.11
(1,132)	1:49:A:LYS:HB2	1:52:A:THR:HB	1	0.11
(1,132)	1:49:A:LYS:HB3	1:52:A:THR:HB	1	0.11
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD2	2	0.11
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD3	2	0.11
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD2	8	0.11
(1,85)	1:44:A:ILE:HB	1:48:A:LYS:HD3	8	0.11
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG2	7	0.11
(1,64)	1:50:A:GLU:H	1:50:A:GLU:HG3	7	0.11
(1,56)	1:172:A:ILE:HB	1:173:A:GLU:H	4	0.11
(1,18)	1:25:A:LEU:HB2	1:26:A:VAL:HA	6	0.11
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD12	2	0.1
(1,1573)	1:129:A:GLY:HA2	1:131:A:ILE:HD13	2	0.1
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD11	2	0.1
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD12	2	0.1
(1,1573)	1:129:A:GLY:HA3	1:131:A:ILE:HD13	2	0.1
(1,1538)	1:118:A:MET:HA	1:122:A:VAL:HG11	3	0.1
(1,1538)	1:118:A:MET:HA	1:122:A:VAL:HG12	3	0.1
(1,1538)	1:118:A:MET:HA	1:122:A:VAL:HG13	3	0.1
(1,1538)	1:118:A:MET:HA	1:122:A:VAL:HG21	3	0.1
(1,1538)	1:118:A:MET:HA	1:122:A:VAL:HG22	3	0.1
(1,1538)	1:118:A:MET:HA	1:122:A:VAL:HG23	3	0.1
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD11	2	0.1
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD12	2	0.1
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD13	2	0.1
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD21	2	0.1
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD22	2	0.1
(1,1536)	1:118:A:MET:HA	1:119:A:LEU:HD23	2	0.1
(1,1527)	1:115:A:PHE:HE1	1:137:A:VAL:HG11	10	0.1
(1,1527)	1:115:A:PHE:HE1	1:137:A:VAL:HG12	10	0.1
(1,1527)	1:115:A:PHE:HE1	1:137:A:VAL:HG13	10	0.1
(1,1527)	1:115:A:PHE:HE1	1:137:A:VAL:HG21	10	0.1
(1,1527)	1:115:A:PHE:HE1	1:137:A:VAL:HG22	10	0.1
(1,1527)	1:115:A:PHE:HE1	1:137:A:VAL:HG23	10	0.1
(1,1527)	1:115:A:PHE:HE2	1:137:A:VAL:HG11	10	0.1
(1,1527)	1:115:A:PHE:HE2	1:137:A:VAL:HG12	10	0.1
(1,1527)	1:115:A:PHE:HE2	1:137:A:VAL:HG13	10	0.1
(1,1527)	1:115:A:PHE:HE2	1:137:A:VAL:HG21	10	0.1
(1,1527)	1:115:A:PHE:HE2	1:137:A:VAL:HG22	10	0.1
(1,1527)	1:115:A:PHE:HE2	1:137:A:VAL:HG23	10	0.1
(1,1467)	1:97:A:GLU:HG2	1:98:A:GLU:H	9	0.1
(1,1467)	1:97:A:GLU:HG3	1:98:A:GLU:H	9	0.1
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD11	1	0.1
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD12	1	0.1
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD13	1	0.1
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD21	1	0.1
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD22	1	0.1
(1,1379)	1:61:A:PHE:HA	1:64:A:LEU:HD23	1	0.1
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD1	3	0.1
(1,1360)	1:56:A:VAL:HG11	1:58:A:PHE:HD2	3	0.1
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD1	3	0.1
(1,1360)	1:56:A:VAL:HG12	1:58:A:PHE:HD2	3	0.1
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD1	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1360)	1:56:A:VAL:HG13	1:58:A:PHE:HD2	3	0.1
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD1	3	0.1
(1,1360)	1:56:A:VAL:HG21	1:58:A:PHE:HD2	3	0.1
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD1	3	0.1
(1,1360)	1:56:A:VAL:HG22	1:58:A:PHE:HD2	3	0.1
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD1	3	0.1
(1,1360)	1:56:A:VAL:HG23	1:58:A:PHE:HD2	3	0.1
(1,1305)	1:40:A:LEU:HD11	1:91:A:PHE:HA	7	0.1
(1,1305)	1:40:A:LEU:HD12	1:91:A:PHE:HA	7	0.1
(1,1305)	1:40:A:LEU:HD13	1:91:A:PHE:HA	7	0.1
(1,1305)	1:40:A:LEU:HD21	1:91:A:PHE:HA	7	0.1
(1,1305)	1:40:A:LEU:HD22	1:91:A:PHE:HA	7	0.1
(1,1305)	1:40:A:LEU:HD23	1:91:A:PHE:HA	7	0.1
(1,1209)	1:64:A:LEU:HD21	1:67:A:GLY:H	3	0.1
(1,1209)	1:64:A:LEU:HD22	1:67:A:GLY:H	3	0.1
(1,1209)	1:64:A:LEU:HD23	1:67:A:GLY:H	3	0.1
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD11	6	0.1
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD12	6	0.1
(1,1172)	1:74:A:GLY:H	1:77:A:LEU:HD13	6	0.1
(1,1127)	1:171:A:ASN:H	1:172:A:ILE:HB	9	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD11	4	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD12	4	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD13	4	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD11	6	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD12	6	0.1
(1,882)	1:60:A:ALA:H	1:64:A:LEU:HD13	6	0.1
(1,858)	1:120:A:GLU:HB2	1:123:A:GLU:H	1	0.1
(1,858)	1:120:A:GLU:HB3	1:123:A:GLU:H	1	0.1
(1,673)	1:80:A:ALA:HA	1:83:A:GLN:HB3	6	0.1
(1,661)	1:157:A:ALA:HA	1:159:A:ILE:H	1	0.1
(1,622)	1:44:A:ILE:HD11	1:85:A:ILE:H	2	0.1
(1,622)	1:44:A:ILE:HD12	1:85:A:ILE:H	2	0.1
(1,622)	1:44:A:ILE:HD13	1:85:A:ILE:H	2	0.1
(1,613)	1:116:A:ASP:HA	1:119:A:LEU:HB3	4	0.1
(1,483)	1:47:A:ILE:HG12	1:84:A:ALA:HB1	7	0.1
(1,483)	1:47:A:ILE:HG12	1:84:A:ALA:HB2	7	0.1
(1,483)	1:47:A:ILE:HG12	1:84:A:ALA:HB3	7	0.1
(1,483)	1:47:A:ILE:HG13	1:84:A:ALA:HB1	7	0.1
(1,483)	1:47:A:ILE:HG13	1:84:A:ALA:HB2	7	0.1
(1,483)	1:47:A:ILE:HG13	1:84:A:ALA:HB3	7	0.1
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG21	4	0.1
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG22	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:141:A:SER:HA	1:146:A:ILE:HG23	4	0.1
(1,430)	1:113:A:ALA:HB1	1:116:A:ASP:H	1	0.1
(1,430)	1:113:A:ALA:HB2	1:116:A:ASP:H	1	0.1
(1,430)	1:113:A:ALA:HB3	1:116:A:ASP:H	1	0.1
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG2	10	0.1
(1,342)	1:148:A:THR:HG21	1:151:A:ARG:HG3	10	0.1
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG2	10	0.1
(1,342)	1:148:A:THR:HG22	1:151:A:ARG:HG3	10	0.1
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG2	10	0.1
(1,342)	1:148:A:THR:HG23	1:151:A:ARG:HG3	10	0.1
(1,270)	1:133:A:LEU:HD11	1:165:A:VAL:HB	4	0.1
(1,270)	1:133:A:LEU:HD12	1:165:A:VAL:HB	4	0.1
(1,270)	1:133:A:LEU:HD13	1:165:A:VAL:HB	4	0.1
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG2	5	0.1
(1,240)	1:46:A:LYS:H	1:48:A:LYS:HG3	5	0.1
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG2	9	0.1
(1,221)	1:148:A:THR:HA	1:151:A:ARG:HG3	9	0.1
(1,181)	1:41:A:LYS:HD2	1:120:A:GLU:HB2	1	0.1
(1,181)	1:41:A:LYS:HD2	1:120:A:GLU:HB3	1	0.1
(1,181)	1:41:A:LYS:HD3	1:120:A:GLU:HB2	1	0.1
(1,181)	1:41:A:LYS:HD3	1:120:A:GLU:HB3	1	0.1
(1,155)	1:51:A:ALA:HB1	1:56:A:VAL:HB	8	0.1
(1,155)	1:51:A:ALA:HB2	1:56:A:VAL:HB	8	0.1
(1,155)	1:51:A:ALA:HB3	1:56:A:VAL:HB	8	0.1
(1,153)	1:82:A:VAL:HB	1:167:A:LYS:HG2	9	0.1
(1,153)	1:82:A:VAL:HB	1:167:A:LYS:HG3	9	0.1
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	3	0.1
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	3	0.1
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	3	0.1
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	3	0.1
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE2	9	0.1
(1,139)	1:38:A:LYS:HB2	1:41:A:LYS:HE3	9	0.1
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE2	9	0.1
(1,139)	1:38:A:LYS:HB3	1:41:A:LYS:HE3	9	0.1
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE2	3	0.1
(1,25)	1:41:A:LYS:HB2	1:41:A:LYS:HE3	3	0.1
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE2	3	0.1
(1,25)	1:41:A:LYS:HB3	1:41:A:LYS:HE3	3	0.1

10 Dihedral-angle violation analysis

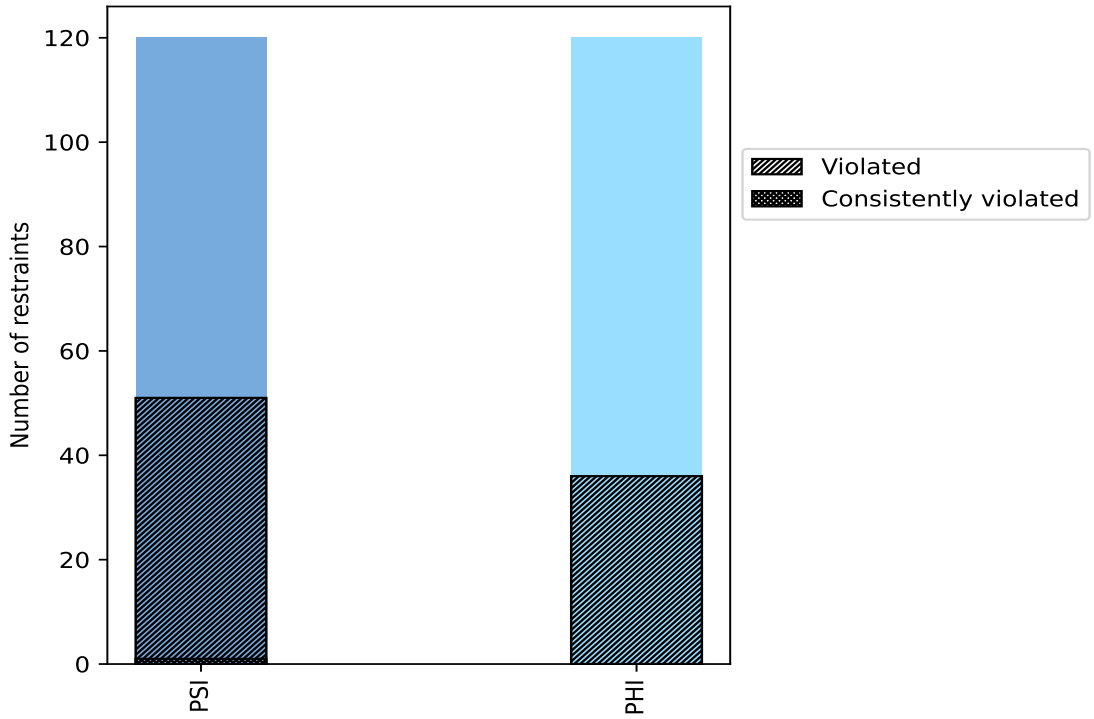
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	120	50.0	51	42.5	21.2	1	0.8	0.4
PHI	120	50.0	36	30.0	15.0	0	0.0	0.0
Total	240	100.0	87	36.2	36.2	1	0.4	0.4

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



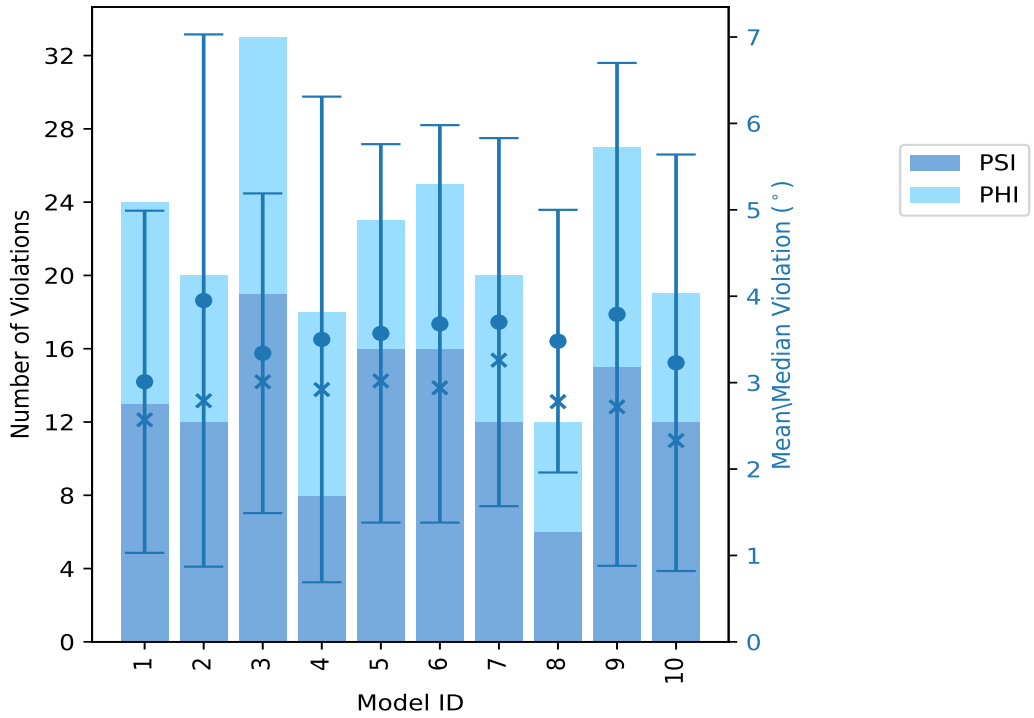
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	13	11	24	3.01	10.49	1.98	2.57
2	12	8	20	3.95	14.4	3.08	2.79
3	19	14	33	3.34	9.92	1.85	3.01
4	8	10	18	3.5	13.79	2.81	2.92
5	16	7	23	3.57	9.86	2.19	3.02
6	16	9	25	3.68	10.64	2.3	2.94
7	12	8	20	3.7	9.02	2.13	3.26
8	6	6	12	3.48	6.54	1.52	2.78
9	15	12	27	3.79	14.2	2.91	2.72
10	12	7	19	3.23	9.91	2.41	2.33

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

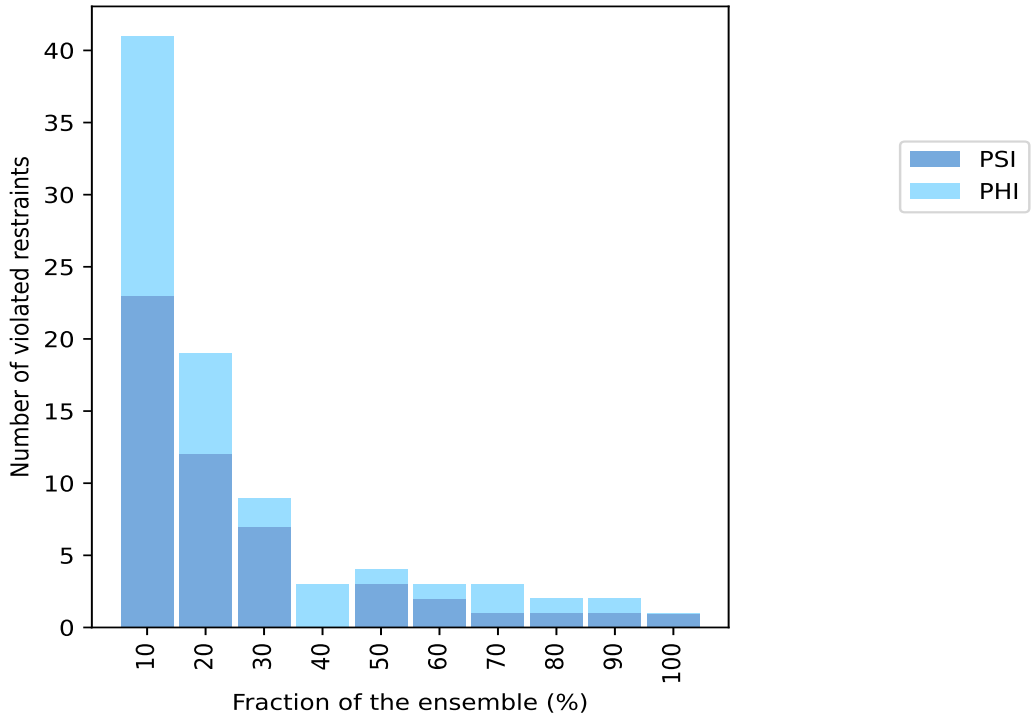
10.3 Dihedral-angle violation statistics for the ensemble (i)

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	
PSI	PHI	Total	Count[1]	%
23	18	41	1	10.0
12	7	19	2	20.0
7	2	9	3	30.0
0	3	3	4	40.0
3	1	4	5	50.0
2	1	3	6	60.0
1	2	3	7	70.0
1	1	2	8	80.0
1	1	2	9	90.0
1	0	1	10	100.0

[1] Number of models with violations

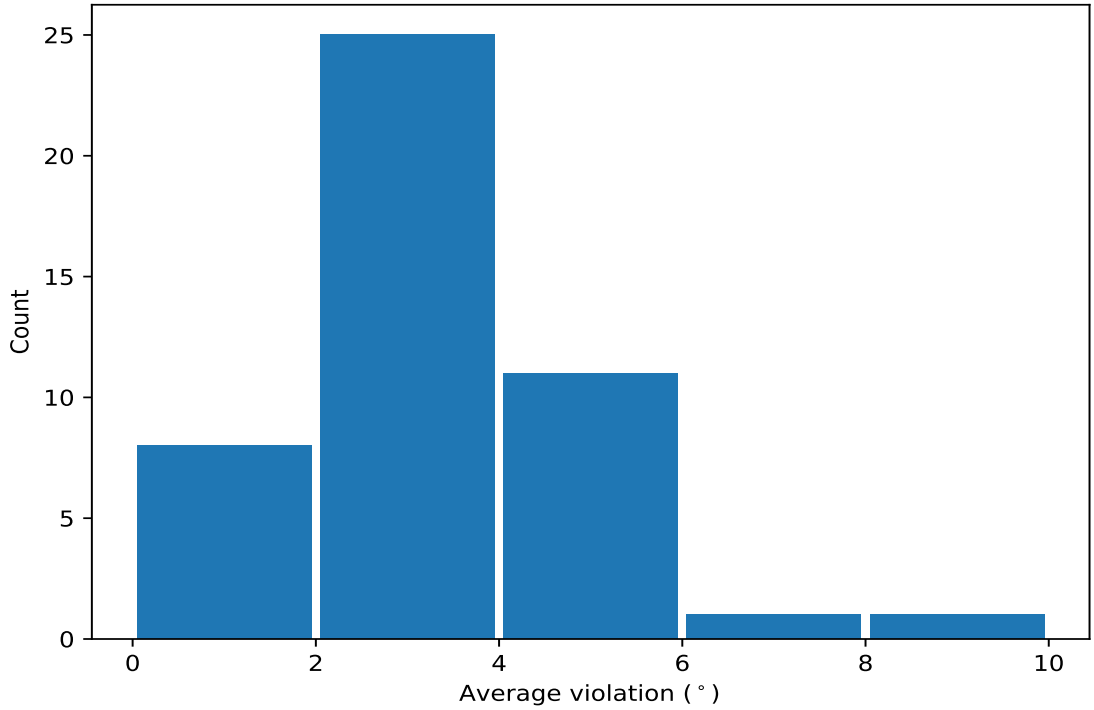
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	10	9.84	2.84	9.91
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	9	4.74	2.32	4.95
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	9	3.31	1.85	3.4
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	8	3.37	1.25	3.26
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	8	2.34	1.38	1.55
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	7	5.66	1.74	5.9
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	7	2.92	1.13	2.87
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	7	2.49	0.9	2.61
(1,88)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ILE:N	6	4.99	1.48	4.57
(1,172)	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1:129:A:GLY:N	6	4.53	1.71	4.77
(1,83)	1:81:A:LYS:C	1:82:A:VAL:N	1:82:A:VAL:CA	1:82:A:VAL:C	6	2.86	2.17	1.8
(1,224)	1:164:A:LYS:N	1:164:A:LYS:CA	1:164:A:LYS:C	1:165:A:VAL:N	5	3.04	0.97	3.53
(1,18)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASP:N	5	2.77	1.62	1.73

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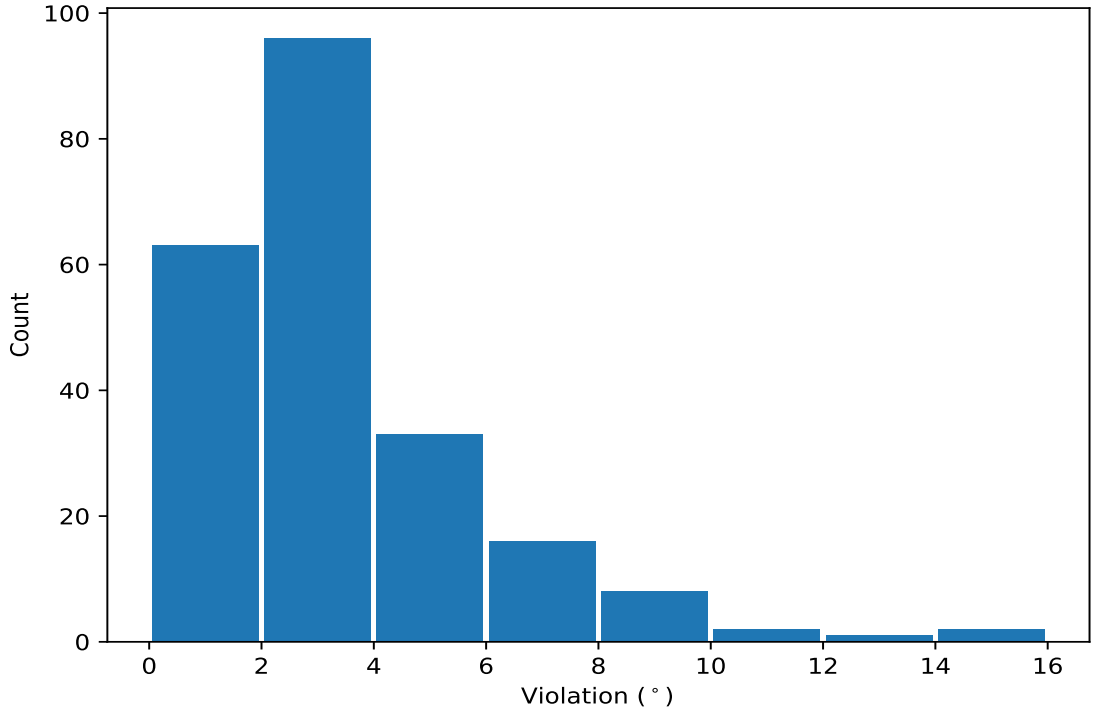
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,171)	1:127:A:ASP:C	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	5	2.23	0.93	2.08
(1,168)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ASP:N	5	2.16	0.26	2.24
(1,175)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	4	4.87	2.59	4.76
(1,173)	1:128:A:VAL:C	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	4	3.78	0.39	3.64
(1,195)	1:142:A:LYS:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	4	2.47	1.34	1.92
(1,174)	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	1:130:A:ILE:N	3	7.17	5.11	3.62
(1,225)	1:164:A:LYS:C	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	3	4.65	1.76	3.85
(1,36)	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	1:48:A:LYS:N	3	4.57	2.26	3.28
(1,48)	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	1:55:A:GLY:N	3	3.28	1.51	2.33
(1,22)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:LYS:N	3	2.48	0.9	3.02
(1,202)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:ALA:N	3	2.45	0.62	2.83
(1,198)	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	1:152:A:LEU:N	3	2.29	0.84	2.1
(1,190)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:SER:N	3	1.95	0.65	2.2
(1,161)	1:122:A:VAL:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	3	1.74	0.46	1.63
(1,120)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:LEU:N	2	5.36	2.71	5.36
(1,170)	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	1:128:A:VAL:N	2	4.3	1.46	4.3
(1,23)	1:40:A:LEU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	2	4.16	0.24	4.16
(1,82)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:VAL:N	2	4.08	0.9	4.08
(1,30)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:LEU:N	2	3.96	2.41	3.96
(1,13)	1:35:A:SER:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	2	3.7	0.62	3.7
(1,26)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:LYS:N	2	3.28	1.27	3.28
(1,42)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:ALA:N	2	3.16	0.12	3.16
(1,33)	1:45:A:LEU:C	1:46:A:LYS:N	1:46:A:LYS:CA	1:46:A:LYS:C	2	3.01	0.96	3.01
(1,73)	1:76:A:ALA:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	2	2.94	0.36	2.94
(1,78)	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	1:80:A:ALA:N	2	2.81	1.11	2.81
(1,234)	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	1:170:A:GLN:N	2	2.74	0.08	2.74
(1,5)	1:30:A:ASN:C	1:31:A:ALA:N	1:31:A:ALA:CA	1:31:A:ALA:C	2	2.66	0.86	2.66
(1,158)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:VAL:N	2	1.98	0.63	1.98
(1,57)	1:59:A:GLU:C	1:60:A:ALA:N	1:60:A:ALA:CA	1:60:A:ALA:C	2	1.88	0.27	1.88
(1,72)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:LEU:N	2	1.88	0.1	1.88
(1,240)	1:182:A:LYS:N	1:182:A:LYS:CA	1:182:A:LYS:C	1:183:A:SER:N	2	1.65	0.07	1.65
(1,74)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:ARG:N	2	1.38	0.15	1.38
(1,125)	1:104:A:GLU:C	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	2	1.29	0.27	1.29

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

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 (°)
(1,174)	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	1:130:A:ILE:N	2	14.4
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	9	14.2
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	4	13.79
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	6	10.64
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	1	10.49
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	3	9.92
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	10	9.91
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	5	9.86
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	7	9.02
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	10	9.0
(1,175)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	7	8.64
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	6	8.28
(1,120)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:LEU:N	5	8.07
(1,28)	1:43:A:LYS:N	1:43:A:LYS:CA	1:43:A:LYS:C	1:44:A:ILE:N	9	7.8
(1,36)	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	1:48:A:LYS:N	2	7.75
(1,83)	1:81:A:LYS:C	1:82:A:VAL:N	1:82:A:VAL:CA	1:82:A:VAL:C	9	7.59
(1,88)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ILE:N	9	7.29
(1,225)	1:164:A:LYS:C	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	2	7.09
(1,172)	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1:129:A:GLY:N	3	6.98
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	3	6.64
(1,88)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ILE:N	6	6.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	3	6.55
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	8	6.54
(1,30)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:LEU:N	2	6.37
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	6	6.22
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	9	6.19
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	1	6.16
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	2	6.15
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	9	6.06
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	9	5.9
(1,172)	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1:129:A:GLY:N	5	5.89
(1,18)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASP:N	7	5.88
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	6	5.84
(1,170)	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	1:128:A:VAL:N	5	5.76
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	5	5.51
(1,48)	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	1:55:A:GLY:N	4	5.41
(1,45)	1:51:A:ALA:C	1:52:A:THR:N	1:52:A:THR:CA	1:52:A:THR:C	8	5.39
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	7	5.16
(1,82)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:VAL:N	8	4.99
(1,172)	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1:129:A:GLY:N	10	4.95
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	1	4.95
(1,175)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	8	4.85
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	7	4.75
(1,195)	1:142:A:LYS:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	3	4.74
(1,88)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ILE:N	4	4.72
(1,175)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	9	4.67
(1,147)	1:115:A:PHE:C	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	5	4.66
(1,76)	1:78:A:ARG:N	1:78:A:ARG:CA	1:78:A:ARG:C	1:79:A:GLU:N	9	4.63
(1,172)	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1:129:A:GLY:N	6	4.58
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	6	4.55
(1,26)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:LYS:N	7	4.55
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	3	4.46
(1,173)	1:128:A:VAL:C	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	6	4.43
(1,88)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ILE:N	1	4.43
(1,219)	1:161:A:ASN:C	1:162:A:GLN:N	1:162:A:GLN:CA	1:162:A:GLN:C	4	4.4
(1,23)	1:40:A:LEU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	4	4.4
(1,13)	1:35:A:SER:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	10	4.32
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	6	4.21
(1,224)	1:164:A:LYS:N	1:164:A:LYS:CA	1:164:A:LYS:C	1:165:A:VAL:N	2	4.16
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1	4.12
(1,32)	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1:46:A:LYS:N	9	4.12
(1,160)	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1:123:A:GLU:N	2	4.07
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	5	3.98
(1,33)	1:45:A:LEU:C	1:46:A:LYS:N	1:46:A:LYS:CA	1:46:A:LYS:C	2	3.97
(1,23)	1:40:A:LEU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	5	3.93
(1,78)	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	1:80:A:ALA:N	3	3.92
(1,50)	1:55:A:GLY:N	1:55:A:GLY:CA	1:55:A:GLY:C	1:56:A:VAL:N	4	3.9
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	6	3.88
(1,225)	1:164:A:LYS:C	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	3	3.85
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	4	3.79
(1,224)	1:164:A:LYS:N	1:164:A:LYS:CA	1:164:A:LYS:C	1:165:A:VAL:N	7	3.75
(1,173)	1:128:A:VAL:C	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	7	3.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	7	3.75
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	5	3.69
(1,174)	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	1:130:A:ILE:N	10	3.62
(1,171)	1:127:A:ASP:C	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	10	3.55
(1,224)	1:164:A:LYS:N	1:164:A:LYS:CA	1:164:A:LYS:C	1:165:A:VAL:N	5	3.53
(1,173)	1:128:A:VAL:C	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	8	3.53
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1	3.52
(1,5)	1:30:A:ASN:C	1:31:A:ALA:N	1:31:A:ALA:CA	1:31:A:ALA:C	4	3.52
(1,77)	1:78:A:ARG:C	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	3	3.51
(1,192)	1:141:A:SER:N	1:141:A:SER:CA	1:141:A:SER:C	1:142:A:LYS:N	3	3.49
(1,174)	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	1:130:A:ILE:N	7	3.49
(1,154)	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	1:120:A:GLU:N	3	3.48
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	4	3.47
(1,88)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ILE:N	5	3.45
(1,173)	1:128:A:VAL:C	1:129:A:GLY:N	1:129:A:GLY:CA	1:129:A:GLY:C	3	3.43
(1,88)	1:84:A:ALA:N	1:84:A:ALA:CA	1:84:A:ALA:C	1:85:A:ILE:N	10	3.41
(1,198)	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	1:152:A:LEU:N	3	3.4
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	10	3.4
(1,73)	1:76:A:ALA:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1	3.31
(1,42)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:ALA:N	6	3.28
(1,36)	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	1:48:A:LYS:N	6	3.28
(1,112)	1:96:A:GLU:N	1:96:A:GLU:CA	1:96:A:GLU:C	1:97:A:GLU:N	3	3.21
(1,22)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:LYS:N	1	3.21
(1,82)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:VAL:N	3	3.18
(1,13)	1:35:A:SER:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	9	3.09
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	3	3.06
(1,181)	1:135:A:ALA:C	1:136:A:ARG:N	1:136:A:ARG:CA	1:136:A:ARG:C	9	3.05
(1,42)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:ALA:N	7	3.04
(1,22)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:LYS:N	5	3.02
(1,225)	1:164:A:LYS:C	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	7	3.01
(1,171)	1:127:A:ASP:C	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	3	3.01
(1,83)	1:81:A:LYS:C	1:82:A:VAL:N	1:82:A:VAL:CA	1:82:A:VAL:C	2	2.98
(1,202)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:ALA:N	5	2.95
(1,8)	1:32:A:ALA:N	1:32:A:ALA:CA	1:32:A:ALA:C	1:33:A:LEU:N	6	2.94
(1,204)	1:154:A:ALA:N	1:154:A:ALA:CA	1:154:A:ALA:C	1:155:A:ALA:N	2	2.9
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	8	2.89
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	10	2.87
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	3	2.87
(1,18)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASP:N	9	2.87
(1,170)	1:127:A:ASP:N	1:127:A:ASP:CA	1:127:A:ASP:C	1:128:A:VAL:N	1	2.84
(1,202)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:ALA:N	3	2.83
(1,234)	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	1:170:A:GLN:N	6	2.82
(1,172)	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1:129:A:GLY:N	1	2.81
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	1	2.74
(1,20)	1:39:A:ASP:N	1:39:A:ASP:CA	1:39:A:ASP:C	1:40:A:LEU:N	3	2.74
(1,64)	1:69:A:LYS:N	1:69:A:LYS:CA	1:69:A:LYS:C	1:70:A:VAL:N	7	2.73
(1,176)	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	1:131:A:ILE:N	5	2.72
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	1	2.72
(1,115)	1:97:A:GLU:C	1:98:A:GLU:N	1:98:A:GLU:CA	1:98:A:GLU:C	9	2.72
(1,179)	1:134:A:LYS:C	1:135:A:ALA:N	1:135:A:ALA:CA	1:135:A:ALA:C	2	2.68
(1,36)	1:47:A:ILE:N	1:47:A:ILE:CA	1:47:A:ILE:C	1:48:A:LYS:N	3	2.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	8	2.68
(1,234)	1:169:A:LYS:N	1:169:A:LYS:CA	1:169:A:LYS:C	1:170:A:GLN:N	3	2.66
(1,120)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:LEU:N	7	2.65
(1,158)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:VAL:N	8	2.61
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	5	2.61
(1,190)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:SER:N	6	2.6
(1,73)	1:76:A:ALA:C	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	3	2.58
(1,218)	1:161:A:ASN:N	1:161:A:ASN:CA	1:161:A:ASN:C	1:162:A:GLN:N	6	2.54
(1,140)	1:112:A:LEU:N	1:112:A:LEU:CA	1:112:A:LEU:C	1:113:A:ALA:N	9	2.5
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	8	2.5
(1,95)	1:87:A:GLU:C	1:88:A:THR:N	1:88:A:THR:CA	1:88:A:THR:C	3	2.48
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	7	2.47
(1,168)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ASP:N	1	2.42
(1,168)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ASP:N	8	2.4
(1,161)	1:122:A:VAL:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	4	2.36
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	2	2.36
(1,48)	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	1:55:A:GLY:N	10	2.33
(1,159)	1:121:A:VAL:C	1:122:A:VAL:N	1:122:A:VAL:CA	1:122:A:VAL:C	1	2.31
(1,14)	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	1:37:A:SER:N	2	2.27
(1,168)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ASP:N	6	2.24
(1,164)	1:124:A:SER:N	1:124:A:SER:CA	1:124:A:SER:C	1:125:A:LEU:N	1	2.23
(1,232)	1:168:A:GLU:N	1:168:A:GLU:CA	1:168:A:GLU:C	1:169:A:LYS:N	2	2.21
(1,190)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:SER:N	3	2.2
(1,195)	1:142:A:LYS:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	4	2.16
(1,57)	1:59:A:GLU:C	1:60:A:ALA:N	1:60:A:ALA:CA	1:60:A:ALA:C	10	2.15
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	6	2.13
(1,48)	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	1:55:A:GLY:N	3	2.11
(1,198)	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	1:152:A:LEU:N	9	2.1
(1,171)	1:127:A:ASP:C	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	4	2.08
(1,168)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ASP:N	5	2.05
(1,153)	1:118:A:MET:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	2	2.05
(1,33)	1:45:A:LEU:C	1:46:A:LYS:N	1:46:A:LYS:CA	1:46:A:LYS:C	9	2.05
(1,127)	1:105:A:THR:C	1:106:A:GLY:N	1:106:A:GLY:CA	1:106:A:GLY:C	1	2.04
(1,224)	1:164:A:LYS:N	1:164:A:LYS:CA	1:164:A:LYS:C	1:165:A:VAL:N	9	2.02
(1,26)	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	1:43:A:LYS:N	6	2.0
(1,72)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:LEU:N	3	1.98
(1,172)	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1:129:A:GLY:N	4	1.95
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	8	1.95
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	10	1.94
(1,25)	1:41:A:LYS:C	1:42:A:ASN:N	1:42:A:ASN:CA	1:42:A:ASN:C	10	1.94
(1,83)	1:81:A:LYS:C	1:82:A:VAL:N	1:82:A:VAL:CA	1:82:A:VAL:C	5	1.84
(1,47)	1:53:A:GLY:C	1:54:A:LYS:N	1:54:A:LYS:CA	1:54:A:LYS:C	9	1.81
(1,5)	1:30:A:ASN:C	1:31:A:ALA:N	1:31:A:ALA:CA	1:31:A:ALA:C	2	1.8
(1,72)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:LEU:N	4	1.77
(1,224)	1:164:A:LYS:N	1:164:A:LYS:CA	1:164:A:LYS:C	1:165:A:VAL:N	1	1.75
(1,83)	1:81:A:LYS:C	1:82:A:VAL:N	1:82:A:VAL:CA	1:82:A:VAL:C	1	1.75
(1,18)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASP:N	1	1.73
(1,240)	1:182:A:LYS:N	1:182:A:LYS:CA	1:182:A:LYS:C	1:183:A:SER:N	9	1.72
(1,168)	1:126:A:GLU:N	1:126:A:GLU:CA	1:126:A:GLU:C	1:127:A:ASP:N	4	1.71
(1,78)	1:79:A:GLU:N	1:79:A:GLU:CA	1:79:A:GLU:C	1:80:A:ALA:N	6	1.7
(1,195)	1:142:A:LYS:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	10	1.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,61)	1:67:A:GLY:C	1:68:A:SER:N	1:68:A:SER:CA	1:68:A:SER:C	7	1.69
(1,18)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASP:N	2	1.69
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	5	1.66
(1,18)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:ASP:N	10	1.66
(1,40)	1:49:A:LYS:N	1:49:A:LYS:CA	1:49:A:LYS:C	1:50:A:GLU:N	9	1.65
(1,161)	1:122:A:VAL:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	6	1.63
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	2	1.63
(1,54)	1:57:A:LEU:N	1:57:A:LEU:CA	1:57:A:LEU:C	1:58:A:PHE:N	5	1.62
(1,57)	1:59:A:GLU:C	1:60:A:ALA:N	1:60:A:ALA:CA	1:60:A:ALA:C	6	1.61
(1,240)	1:182:A:LYS:N	1:182:A:LYS:CA	1:182:A:LYS:C	1:183:A:SER:N	1	1.58
(1,58)	1:60:A:ALA:N	1:60:A:ALA:CA	1:60:A:ALA:C	1:61:A:PHE:N	9	1.58
(1,202)	1:153:A:LEU:N	1:153:A:LEU:CA	1:153:A:LEU:C	1:154:A:ALA:N	9	1.57
(1,4)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	3	1.57
(1,125)	1:104:A:GLU:C	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	3	1.56
(1,83)	1:81:A:LYS:C	1:82:A:VAL:N	1:82:A:VAL:CA	1:82:A:VAL:C	7	1.56
(1,197)	1:150:A:GLU:C	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	9	1.55
(1,30)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:LEU:N	7	1.55
(1,74)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:ARG:N	6	1.52
(1,107)	1:93:A:LYS:C	1:94:A:ILE:N	1:94:A:ILE:CA	1:94:A:ILE:C	3	1.51
(1,171)	1:127:A:ASP:C	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	1	1.44
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	8	1.44
(1,83)	1:81:A:LYS:C	1:82:A:VAL:N	1:82:A:VAL:CA	1:82:A:VAL:C	4	1.44
(1,209)	1:156:A:LYS:C	1:157:A:ALA:N	1:157:A:ALA:CA	1:157:A:ALA:C	1	1.41
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	7	1.41
(1,198)	1:151:A:ARG:N	1:151:A:ARG:CA	1:151:A:ARG:C	1:152:A:LEU:N	5	1.38
(1,158)	1:121:A:VAL:N	1:121:A:VAL:CA	1:121:A:VAL:C	1:122:A:VAL:N	1	1.34
(1,138)	1:111:A:PHE:N	1:111:A:PHE:CA	1:111:A:PHE:C	1:112:A:LEU:N	5	1.34
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	9	1.34
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	10	1.34
(1,175)	1:129:A:GLY:C	1:130:A:ILE:N	1:130:A:ILE:CA	1:130:A:ILE:C	6	1.33
(1,195)	1:142:A:LYS:C	1:143:A:ASN:N	1:143:A:ASN:CA	1:143:A:ASN:C	5	1.3
(1,59)	1:66:A:THR:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	3	1.3
(1,205)	1:154:A:ALA:C	1:155:A:ALA:N	1:155:A:ALA:CA	1:155:A:ALA:C	2	1.29
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	2	1.27
(1,161)	1:122:A:VAL:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	9	1.24
(1,106)	1:93:A:LYS:N	1:93:A:LYS:CA	1:93:A:LYS:C	1:94:A:ILE:N	3	1.24
(1,74)	1:77:A:LEU:N	1:77:A:LEU:CA	1:77:A:LEU:C	1:78:A:ARG:N	5	1.23
(1,22)	1:40:A:LEU:N	1:40:A:LEU:CA	1:40:A:LEU:C	1:41:A:LYS:N	10	1.22
(1,239)	1:181:A:ASN:C	1:182:A:LYS:N	1:182:A:LYS:CA	1:182:A:LYS:C	7	1.21
(1,31)	1:44:A:ILE:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	4	1.13
(1,126)	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1:106:A:GLY:N	9	1.11
(1,171)	1:127:A:ASP:C	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	6	1.08
(1,190)	1:140:A:GLU:N	1:140:A:GLU:CA	1:140:A:GLU:C	1:141:A:SER:N	10	1.06
(1,148)	1:116:A:ASP:N	1:116:A:ASP:CA	1:116:A:ASP:C	1:117:A:LEU:N	4	1.05
(1,125)	1:104:A:GLU:C	1:105:A:THR:N	1:105:A:THR:CA	1:105:A:THR:C	1	1.02
(1,10)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:SER:N	10	1.01
(1,89)	1:84:A:ALA:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	3	1.0