



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 01:44 PM EST

PDB ID : 6Q44  
BMRB ID : 27146  
Title : Est3 telomerase subunit in the yeast *Hansenula polymorpha*  
Authors : Mantsyzov, A.B.; Mariasina, S.S.; Petrova, O.A.; Efimov, S.V.; Dontsova, O.A.; Polshakov, V.I.  
Deposited on : 2018-12-05

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

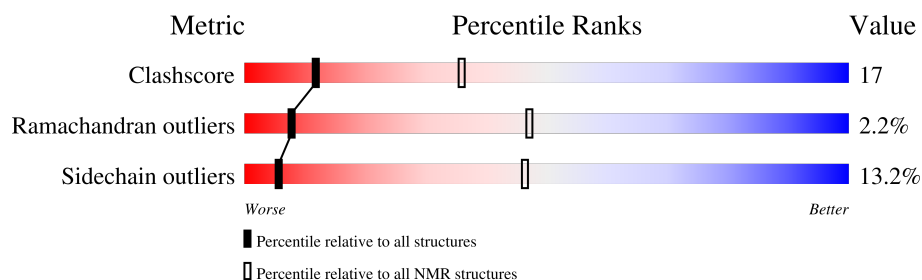
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 80%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	178	

## 2 Ensemble composition and analysis

This entry contains 20 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:23-A:172 (150)	0.86	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 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 7, 8, 9, 10, 12, 13, 15, 16, 18, 19
2	14, 17
Single-model clusters	5; 11; 20

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2882 atoms, of which 1439 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	178	Total	C	H	N	O	S	0
			2882	926	1439	249	261	7	

There are 4 discrepancies between the modelled and reference sequences:

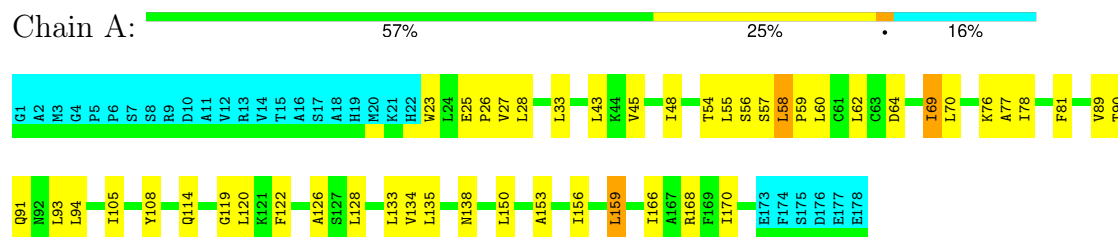
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP W1QJK4
A	2	ALA	-	expression tag	UNP W1QJK4
A	3	MET	-	expression tag	UNP W1QJK4
A	4	GLY	-	expression tag	UNP W1QJK4

## 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: Uncharacterized protein

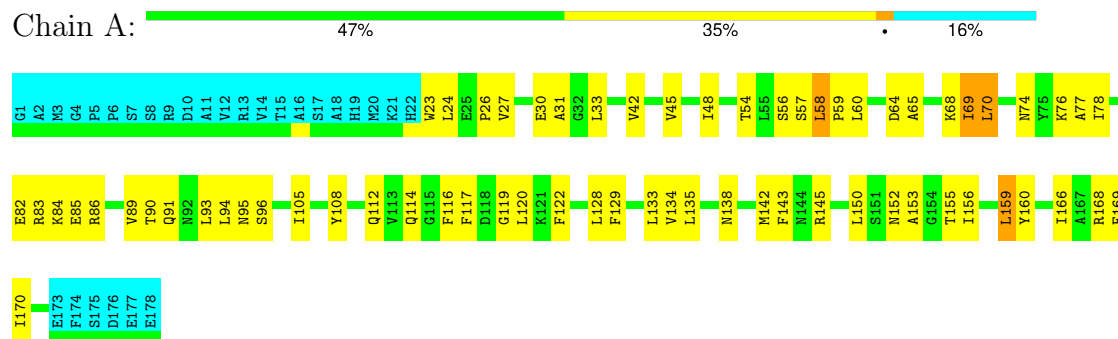


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

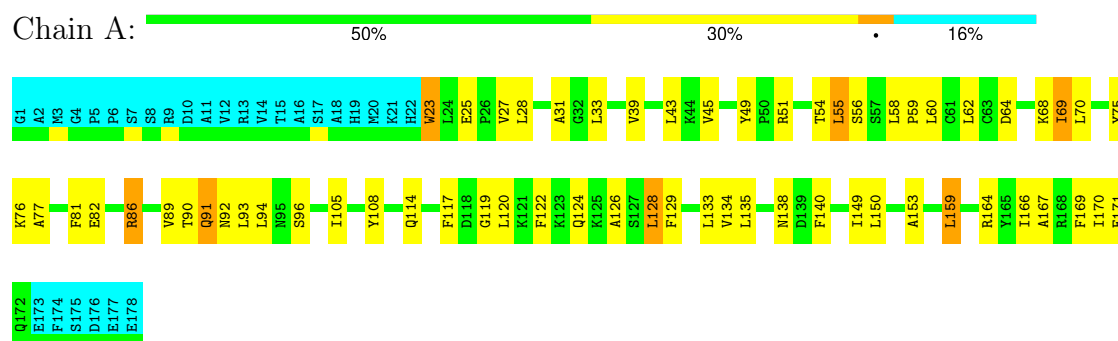
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Uncharacterized protein



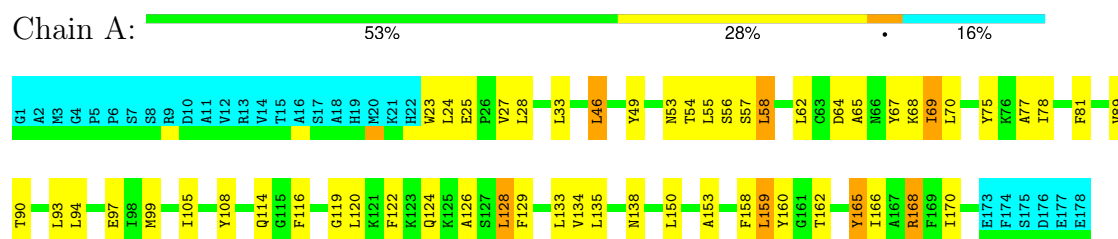
#### 4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein



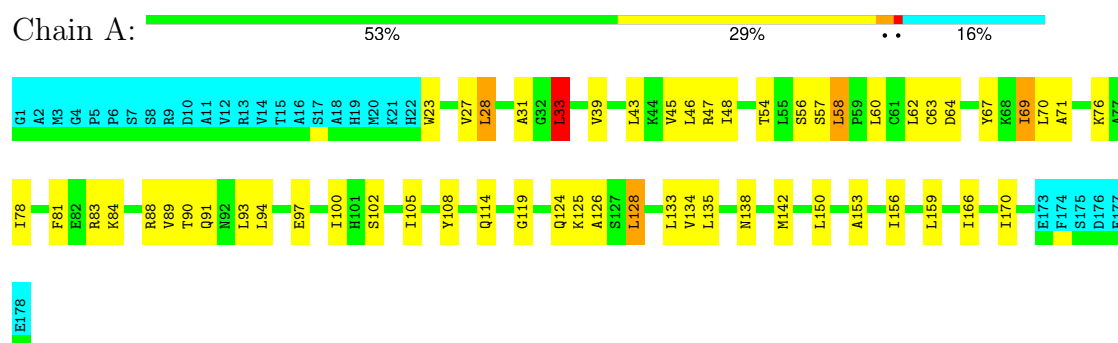
### 4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein



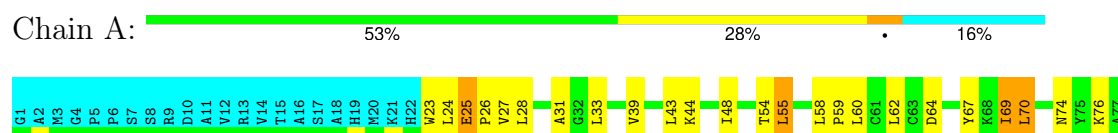
### 4.2.4 Score per residue for model 4

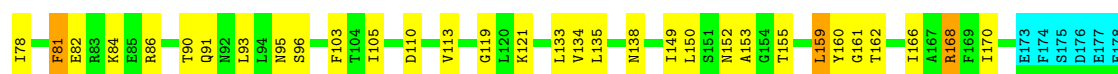
- Molecule 1: Uncharacterized protein



### 4.2.5 Score per residue for model 5

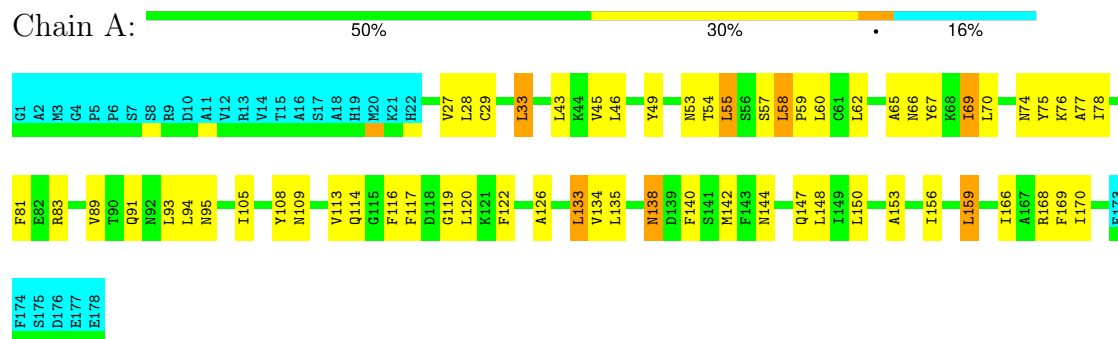
- Molecule 1: Uncharacterized protein





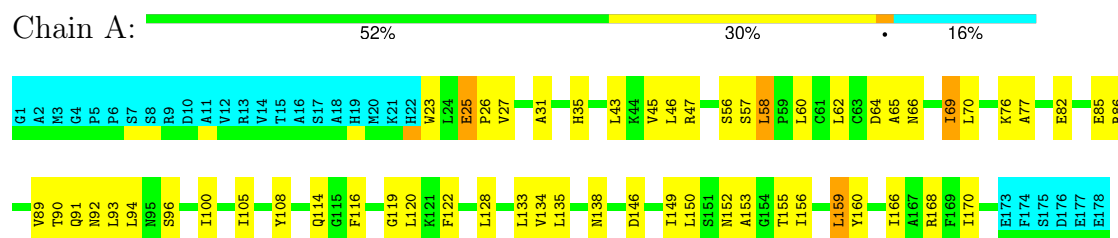
#### 4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein



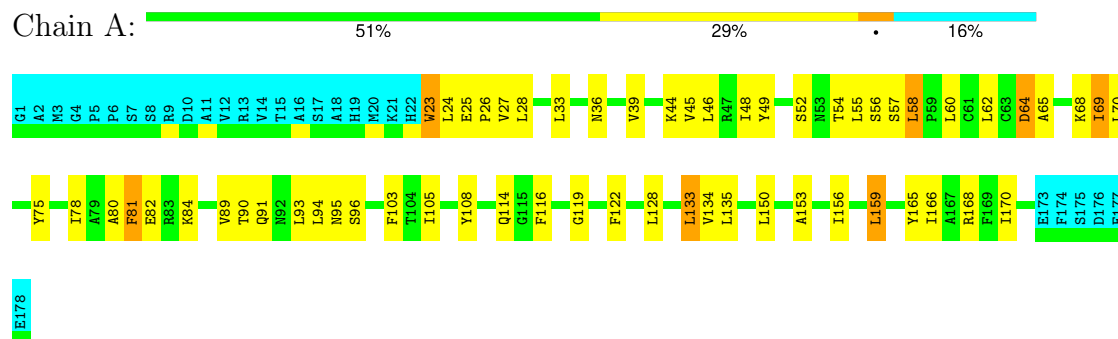
#### 4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



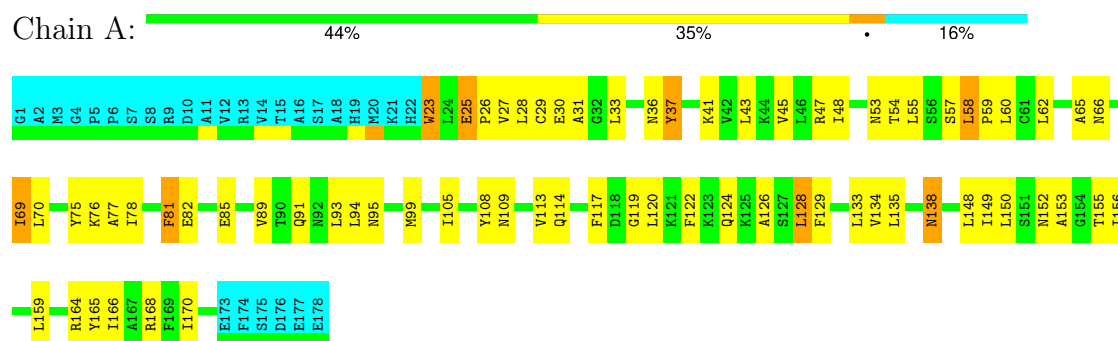
#### 4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



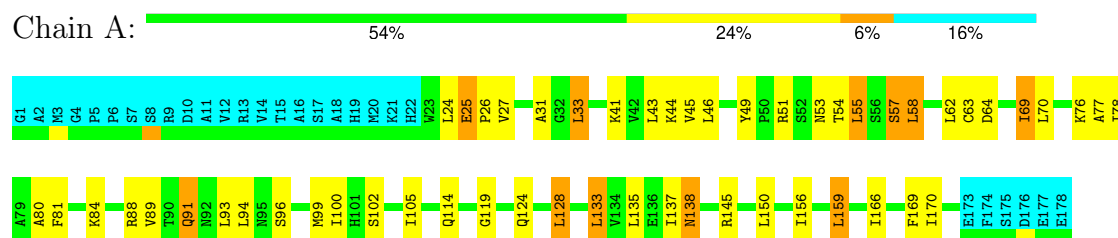
### 4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



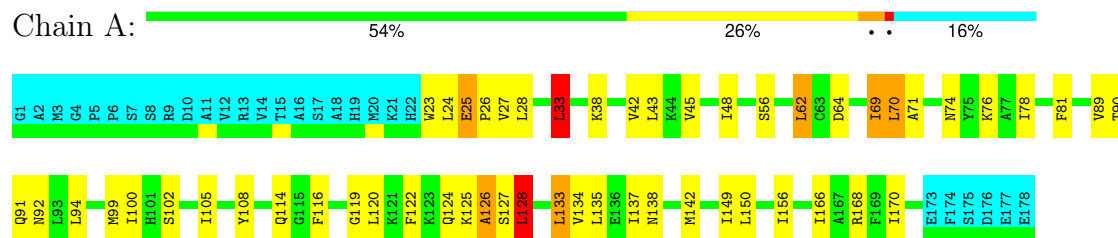
### 4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



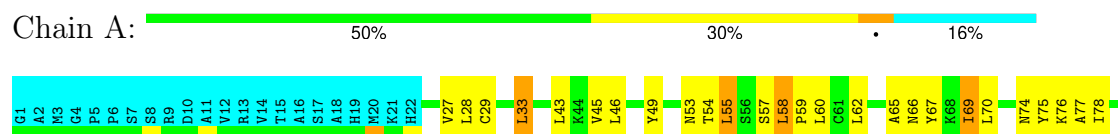
### 4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein

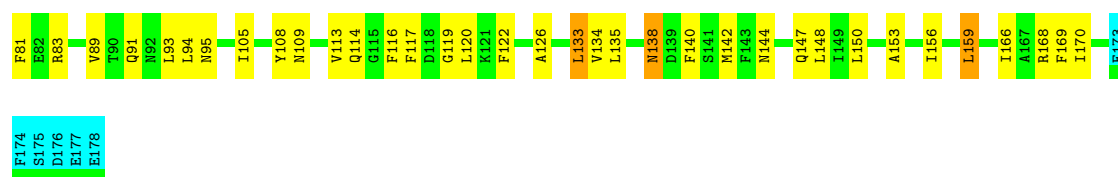


### 4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein

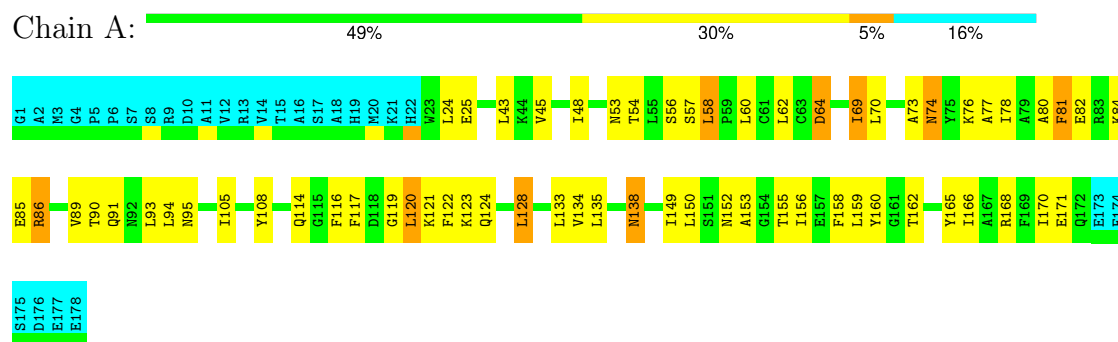






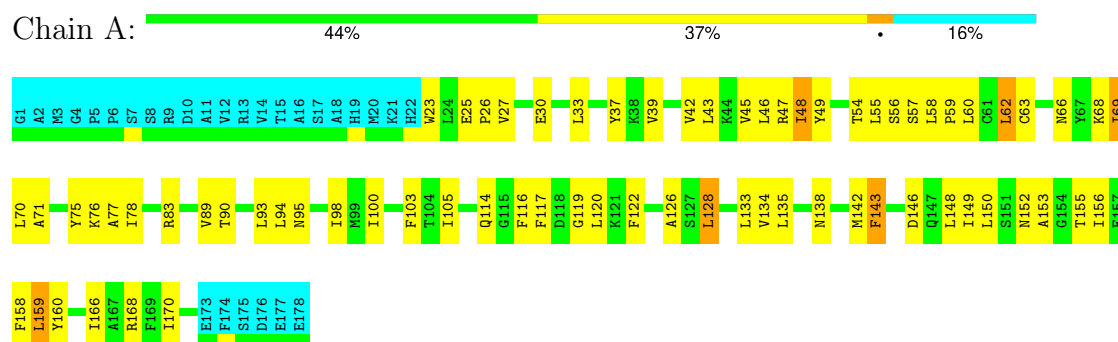
#### 4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



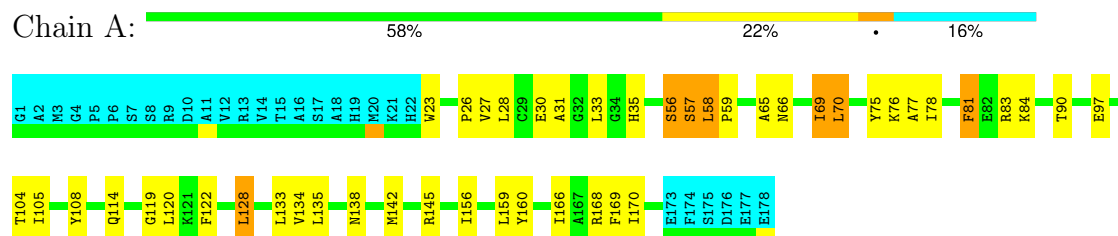
#### 4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



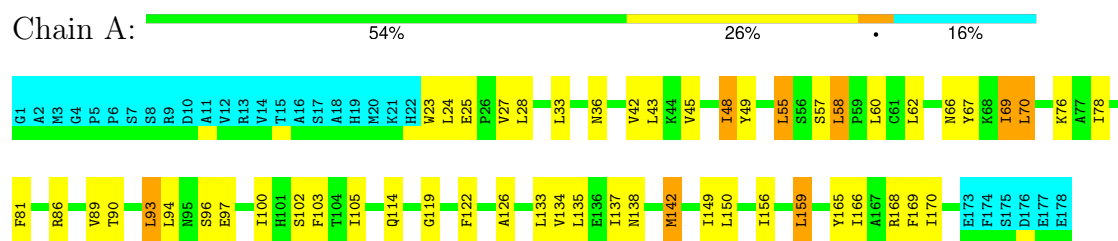
#### 4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



### 4.2.16 Score per residue for model 16

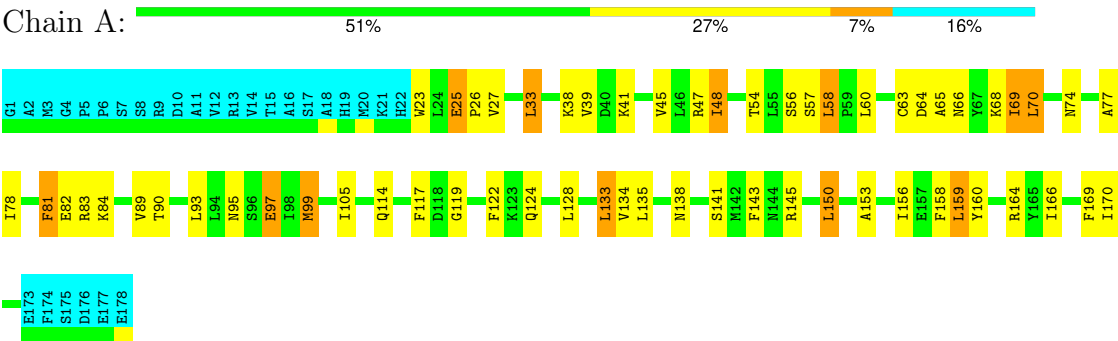
- Molecule 1: Uncharacterized protein



D176  
E177  
E178

4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CNS	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1997
Number of shifts mapped to atoms	1997
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

## 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	1234	1244	1242	43±7
All	All	24680	24880	24840	853

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:166:ILE:HG23	1:A:170:ILE:HD12	1.09	1.20	13	11
1:A:150:LEU:HD23	1:A:153:ALA:HB2	1.02	1.32	17	13
1:A:27:VAL:HG23	1:A:33:LEU:HD13	0.90	1.44	16	10
1:A:33:LEU:HD21	1:A:39:VAL:HG13	0.86	1.45	8	4
1:A:55:LEU:HD12	1:A:78:ILE:HG21	0.85	1.44	6	3
1:A:105:ILE:HD12	1:A:133:LEU:HD21	0.84	1.45	2	15
1:A:33:LEU:HD22	1:A:37:TYR:CD2	0.82	2.09	14	1
1:A:70:LEU:HD21	1:A:122:PHE:CZ	0.81	2.11	17	10
1:A:133:LEU:HD13	1:A:165:TYR:CE2	0.80	2.10	3	1
1:A:55:LEU:HD12	1:A:78:ILE:CG2	0.79	2.07	6	3
1:A:33:LEU:HD11	1:A:39:VAL:HG11	0.78	1.55	4	3
1:A:49:TYR:O	1:A:58:LEU:HD11	0.76	1.81	18	2
1:A:33:LEU:HD13	1:A:37:TYR:CE2	0.76	2.15	14	2
1:A:55:LEU:CD1	1:A:78:ILE:HG21	0.76	2.11	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD23	1:A:37:TYR:HB3	0.75	1.57	18	1
1:A:45:VAL:HG11	1:A:94:LEU:HB3	0.75	1.57	10	11
1:A:152:ASN:O	1:A:155:THR:HG22	0.74	1.82	13	9
1:A:90:THR:HG22	1:A:94:LEU:HD11	0.74	1.60	3	3
1:A:33:LEU:HD13	1:A:37:TYR:CD2	0.74	2.18	19	1
1:A:27:VAL:CG2	1:A:33:LEU:HD13	0.72	2.15	1	5
1:A:93:LEU:HD22	1:A:94:LEU:N	0.72	2.00	16	1
1:A:166:ILE:HG23	1:A:170:ILE:CD1	0.72	2.11	10	3
1:A:113:VAL:HG21	1:A:122:PHE:CD2	0.71	2.19	6	2
1:A:33:LEU:HD11	1:A:39:VAL:CG1	0.71	2.15	4	2
1:A:42:VAL:HG22	1:A:143:PHE:CD1	0.70	2.22	14	2
1:A:60:LEU:HD12	1:A:60:LEU:O	0.69	1.87	5	4
1:A:45:VAL:CG2	1:A:60:LEU:HD13	0.69	2.18	9	8
1:A:62:LEU:HD21	1:A:71:ALA:HB3	0.68	1.62	19	3
1:A:27:VAL:CG2	1:A:33:LEU:HD11	0.68	2.18	14	1
1:A:69:ILE:CG2	1:A:159:LEU:HD13	0.67	2.19	15	4
1:A:166:ILE:HG23	1:A:170:ILE:HG13	0.67	1.67	9	9
1:A:57:SER:HB3	1:A:78:ILE:HG23	0.67	1.65	15	7
1:A:57:SER:C	1:A:58:LEU:HD13	0.67	2.11	16	14
1:A:43:LEU:HD22	1:A:100:ILE:HD11	0.66	1.66	19	3
1:A:47:ARG:O	1:A:48:ILE:HD13	0.66	1.89	17	3
1:A:57:SER:HB2	1:A:78:ILE:HG23	0.66	1.67	9	3
1:A:43:LEU:HD23	1:A:62:LEU:HD11	0.66	1.67	9	1
1:A:129:PHE:CE1	1:A:170:ILE:HG21	0.66	2.26	1	1
1:A:58:LEU:N	1:A:58:LEU:HD13	0.65	2.06	8	7
1:A:159:LEU:HD23	1:A:159:LEU:O	0.65	1.91	9	2
1:A:120:LEU:HD21	1:A:122:PHE:CZ	0.65	2.27	2	7
1:A:80:ALA:HB1	1:A:84:LYS:HE2	0.65	1.68	13	3
1:A:70:LEU:O	1:A:134:VAL:HG13	0.65	1.92	1	10
1:A:70:LEU:HD21	1:A:122:PHE:CE2	0.65	2.26	18	1
1:A:66:ASN:O	1:A:156:ILE:HG23	0.65	1.92	6	8
1:A:27:VAL:HG22	1:A:33:LEU:HD11	0.65	1.68	14	1
1:A:70:LEU:HD21	1:A:122:PHE:CE1	0.64	2.26	14	7
1:A:54:THR:OG1	1:A:58:LEU:HD12	0.64	1.93	20	1
1:A:24:LEU:HD11	1:A:64:ASP:OD2	0.63	1.93	11	2
1:A:27:VAL:O	1:A:31:ALA:HB3	0.63	1.94	2	3
1:A:28:LEU:HD11	1:A:169:PHE:CZ	0.63	2.29	16	1
1:A:166:ILE:CG2	1:A:170:ILE:HD12	0.63	2.12	13	4
1:A:46:LEU:HD11	1:A:150:LEU:HB3	0.62	1.72	7	2
1:A:27:VAL:HG22	1:A:33:LEU:HB2	0.62	1.71	11	4
1:A:105:ILE:HG23	1:A:133:LEU:CD2	0.61	2.24	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ILE:HD13	1:A:135:LEU:CD1	0.61	2.25	10	18
1:A:75:TYR:HA	1:A:78:ILE:HD12	0.61	1.72	8	6
1:A:77:ALA:HB2	1:A:138:ASN:O	0.61	1.96	18	14
1:A:48:ILE:HG21	1:A:90:THR:HB	0.61	1.73	20	7
1:A:128:LEU:HD13	1:A:128:LEU:N	0.61	2.11	13	5
1:A:55:LEU:HD12	1:A:78:ILE:HD13	0.61	1.71	10	2
1:A:55:LEU:HD13	1:A:75:TYR:CD2	0.60	2.31	17	1
1:A:24:LEU:HD21	1:A:64:ASP:OD1	0.60	1.96	5	1
1:A:100:ILE:HG23	1:A:137:ILE:HG23	0.60	1.73	16	4
1:A:27:VAL:HG23	1:A:33:LEU:HD23	0.60	1.72	15	3
1:A:42:VAL:C	1:A:43:LEU:HD22	0.59	2.18	11	2
1:A:23:TRP:O	1:A:27:VAL:HG12	0.59	1.98	15	9
1:A:42:VAL:HG11	1:A:97:GLU:OE2	0.59	1.96	16	1
1:A:131:GLY:CA	1:A:170:ILE:HD11	0.59	2.28	17	1
1:A:89:VAL:HA	1:A:93:LEU:HD12	0.58	1.76	3	12
1:A:159:LEU:HD22	1:A:159:LEU:O	0.58	1.99	7	4
1:A:45:VAL:C	1:A:46:LEU:HD22	0.58	2.17	17	2
1:A:62:LEU:HD11	1:A:69:ILE:HD11	0.58	1.75	17	3
1:A:159:LEU:H	1:A:159:LEU:HD13	0.57	1.58	1	2
1:A:43:LEU:CD2	1:A:100:ILE:HD11	0.57	2.29	7	2
1:A:24:LEU:HD21	1:A:64:ASP:OD2	0.57	1.99	3	1
1:A:28:LEU:HD23	1:A:168:ARG:HG2	0.57	1.76	3	1
1:A:47:ARG:C	1:A:48:ILE:HD13	0.56	2.20	20	4
1:A:89:VAL:HG22	1:A:94:LEU:HG	0.56	1.76	2	1
1:A:55:LEU:HD11	1:A:75:TYR:HE2	0.56	1.59	6	2
1:A:31:ALA:HB1	1:A:33:LEU:HD12	0.56	1.76	18	1
1:A:70:LEU:HD13	1:A:70:LEU:N	0.56	2.15	1	1
1:A:93:LEU:HD13	1:A:93:LEU:H	0.56	1.61	16	1
1:A:81:PHE:CE2	1:A:89:VAL:HG12	0.56	2.36	10	1
1:A:70:LEU:HB2	1:A:134:VAL:HG22	0.56	1.75	11	4
1:A:89:VAL:HG23	1:A:93:LEU:CB	0.56	2.31	20	1
1:A:31:ALA:CB	1:A:33:LEU:HD12	0.55	2.30	18	1
1:A:58:LEU:HD13	1:A:58:LEU:N	0.55	2.17	1	7
1:A:64:ASP:O	1:A:156:ILE:HD11	0.55	2.01	10	2
1:A:127:SER:C	1:A:128:LEU:HD23	0.55	2.22	11	1
1:A:133:LEU:HD11	1:A:169:PHE:CE2	0.55	2.37	6	3
1:A:133:LEU:HD11	1:A:169:PHE:CE1	0.55	2.36	20	1
1:A:45:VAL:CG1	1:A:60:LEU:HD13	0.55	2.31	14	2
1:A:150:LEU:HD21	1:A:156:ILE:CD1	0.54	2.32	16	1
1:A:27:VAL:HG13	1:A:28:LEU:HD23	0.54	1.76	4	2
1:A:60:LEU:HD22	1:A:94:LEU:HD13	0.54	1.80	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ALA:HB1	1:A:84:LYS:CE	0.54	2.32	10	1
1:A:33:LEU:HD21	1:A:39:VAL:CG1	0.54	2.26	8	4
1:A:89:VAL:HG22	1:A:94:LEU:CD2	0.54	2.33	8	10
1:A:69:ILE:H	1:A:69:ILE:HD13	0.54	1.62	1	18
1:A:159:LEU:C	1:A:159:LEU:HD22	0.54	2.23	14	8
1:A:42:VAL:HG22	1:A:143:PHE:HD1	0.54	1.59	14	1
1:A:108:TYR:CD2	1:A:134:VAL:HG21	0.53	2.38	2	4
1:A:56:SER:O	1:A:90:THR:HG23	0.53	2.03	8	12
1:A:46:LEU:HD22	1:A:46:LEU:N	0.53	2.18	3	3
1:A:27:VAL:HG13	1:A:28:LEU:CD2	0.53	2.34	16	1
1:A:43:LEU:HD22	1:A:100:ILE:CD1	0.53	2.33	19	3
1:A:70:LEU:C	1:A:134:VAL:HG13	0.53	2.24	14	3
1:A:27:VAL:HA	1:A:31:ALA:HB3	0.53	1.81	15	4
1:A:149:ILE:HD12	1:A:149:ILE:N	0.53	2.19	9	9
1:A:125:LYS:O	1:A:126:ALA:HB2	0.53	2.03	11	1
1:A:28:LEU:HD21	1:A:169:PHE:CE1	0.53	2.38	19	1
1:A:43:LEU:HD12	1:A:62:LEU:HD12	0.52	1.81	16	1
1:A:28:LEU:HD12	1:A:165:TYR:CE1	0.52	2.39	19	1
1:A:108:TYR:CD1	1:A:134:VAL:HG21	0.52	2.40	6	5
1:A:159:LEU:HD22	1:A:159:LEU:C	0.52	2.25	2	3
1:A:85:GLU:OE2	1:A:93:LEU:HD13	0.52	2.04	9	2
1:A:68:LYS:O	1:A:159:LEU:HD11	0.52	2.05	1	1
1:A:45:VAL:HG23	1:A:60:LEU:HD13	0.52	1.82	4	4
1:A:43:LEU:HD11	1:A:62:LEU:HD13	0.52	1.80	18	3
1:A:64:ASP:O	1:A:156:ILE:HD13	0.52	2.05	1	1
1:A:108:TYR:CG	1:A:134:VAL:HG21	0.52	2.40	8	8
1:A:63:CYS:SG	1:A:150:LEU:HD22	0.52	2.45	19	1
1:A:77:ALA:HB2	1:A:138:ASN:C	0.52	2.25	1	3
1:A:55:LEU:HD11	1:A:75:TYR:CE2	0.52	2.40	6	2
1:A:27:VAL:HG22	1:A:33:LEU:CD1	0.52	2.34	14	1
1:A:58:LEU:N	1:A:58:LEU:HD22	0.51	2.20	16	4
1:A:25:GLU:CB	1:A:26:PRO:HD3	0.51	2.36	9	8
1:A:46:LEU:HD13	1:A:63:CYS:SG	0.51	2.45	10	2
1:A:93:LEU:HD22	1:A:93:LEU:C	0.51	2.25	16	1
1:A:46:LEU:HD22	1:A:63:CYS:SG	0.51	2.46	10	3
1:A:24:LEU:HD11	1:A:64:ASP:CG	0.51	2.26	13	1
1:A:153:ALA:HA	1:A:156:ILE:HD12	0.51	1.83	8	7
1:A:62:LEU:HD11	1:A:69:ILE:CD1	0.51	2.36	17	2
1:A:128:LEU:HD22	1:A:128:LEU:N	0.51	2.20	4	2
1:A:45:VAL:HG21	1:A:60:LEU:HD13	0.51	1.82	9	1
1:A:55:LEU:HB3	1:A:78:ILE:HG21	0.51	1.82	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:HD3	1:A:150:LEU:HD13	0.51	1.83	8	1
1:A:73:ALA:O	1:A:78:ILE:HD11	0.51	2.05	13	1
1:A:55:LEU:CD1	1:A:75:TYR:CE2	0.51	2.94	14	1
1:A:45:VAL:HG12	1:A:94:LEU:O	0.50	2.06	9	3
1:A:46:LEU:HD21	1:A:153:ALA:CB	0.50	2.36	8	1
1:A:69:ILE:HG13	1:A:135:LEU:HD23	0.50	1.83	7	10
1:A:35:HIS:HA	1:A:104:THR:HG23	0.50	1.84	15	1
1:A:45:VAL:HG11	1:A:94:LEU:CB	0.50	2.37	17	6
1:A:58:LEU:H	1:A:58:LEU:HD22	0.50	1.66	13	2
1:A:53:ASN:O	1:A:54:THR:HG22	0.50	2.07	10	5
1:A:23:TRP:HE1	1:A:43:LEU:HD13	0.50	1.67	18	1
1:A:31:ALA:HB3	1:A:33:LEU:HD12	0.50	1.84	4	1
1:A:62:LEU:HD21	1:A:71:ALA:CB	0.50	2.37	14	2
1:A:43:LEU:HD11	1:A:62:LEU:CD1	0.50	2.37	18	4
1:A:60:LEU:CD1	1:A:62:LEU:HD22	0.49	2.37	14	3
1:A:150:LEU:HD21	1:A:156:ILE:HD11	0.49	1.84	16	2
1:A:90:THR:HG22	1:A:94:LEU:CD1	0.49	2.37	19	1
1:A:131:GLY:HA3	1:A:170:ILE:HD11	0.49	1.83	17	1
1:A:97:GLU:HB3	1:A:145:ARG:HB2	0.49	1.83	20	1
1:A:45:VAL:CG2	1:A:48:ILE:HD11	0.49	2.37	18	1
1:A:69:ILE:HG22	1:A:159:LEU:HD13	0.49	1.83	4	3
1:A:23:TRP:CZ2	1:A:43:LEU:HD21	0.49	2.43	11	2
1:A:55:LEU:HD13	1:A:75:TYR:CE2	0.49	2.43	17	1
1:A:158:PHE:O	1:A:162:THR:HG23	0.49	2.08	17	2
1:A:44:LYS:HD2	1:A:150:LEU:HD12	0.49	1.85	19	1
1:A:109:ASN:O	1:A:113:VAL:HG22	0.49	2.07	6	3
1:A:58:LEU:HD22	1:A:58:LEU:H	0.49	1.67	16	2
1:A:28:LEU:HD12	1:A:169:PHE:CE1	0.48	2.43	15	1
1:A:90:THR:HA	1:A:94:LEU:HD12	0.48	1.84	2	2
1:A:74:ASN:O	1:A:78:ILE:HG13	0.48	2.08	20	7
1:A:128:LEU:HD22	1:A:129:PHE:N	0.48	2.24	2	2
1:A:24:LEU:O	1:A:27:VAL:HG12	0.48	2.08	16	3
1:A:135:LEU:N	1:A:135:LEU:HD22	0.48	2.24	10	13
1:A:43:LEU:HD23	1:A:62:LEU:CD1	0.48	2.39	19	2
1:A:33:LEU:HD22	1:A:103:PHE:CZ	0.47	2.43	8	2
1:A:57:SER:HA	1:A:90:THR:HG21	0.47	1.86	19	1
1:A:43:LEU:HD13	1:A:64:ASP:OD1	0.47	2.10	10	1
1:A:103:PHE:CD2	1:A:135:LEU:HD12	0.47	2.44	5	1
1:A:81:PHE:CD1	1:A:82:GLU:N	0.47	2.83	13	3
1:A:45:VAL:HG22	1:A:94:LEU:HB3	0.47	1.87	16	2
1:A:82:GLU:O	1:A:86:ARG:HA	0.47	2.10	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:PHE:CZ	1:A:89:VAL:HG23	0.47	2.45	2	1
1:A:54:THR:HG22	1:A:55:LEU:N	0.47	2.25	5	2
1:A:69:ILE:HG22	1:A:159:LEU:HG	0.47	1.86	6	3
1:A:62:LEU:CD2	1:A:71:ALA:HB3	0.47	2.40	14	2
1:A:105:ILE:HD13	1:A:135:LEU:HD11	0.47	1.87	11	1
1:A:159:LEU:HD22	1:A:160:TYR:N	0.46	2.25	1	1
1:A:67:TYR:CB	1:A:159:LEU:HD12	0.46	2.38	4	1
1:A:105:ILE:HG21	1:A:169:PHE:CE2	0.46	2.44	1	2
1:A:128:LEU:HD22	1:A:128:LEU:H	0.46	1.69	4	2
1:A:99:MET:N	1:A:141:SER:O	0.46	2.48	20	1
1:A:147:GLN:C	1:A:148:LEU:HD22	0.46	2.31	6	2
1:A:81:PHE:CE2	1:A:82:GLU:CG	0.46	2.99	9	1
1:A:48:ILE:HD12	1:A:94:LEU:HD12	0.46	1.87	16	1
1:A:150:LEU:CD2	1:A:153:ALA:HB2	0.46	2.34	13	1
1:A:100:ILE:HG23	1:A:137:ILE:CG2	0.46	2.40	16	1
1:A:128:LEU:HD13	1:A:128:LEU:H	0.46	1.70	2	3
1:A:66:ASN:C	1:A:156:ILE:HG23	0.46	2.30	15	1
1:A:69:ILE:HD13	1:A:69:ILE:N	0.46	2.26	16	15
1:A:24:LEU:HD11	1:A:64:ASP:HB2	0.46	1.86	1	1
1:A:27:VAL:HG23	1:A:33:LEU:HD11	0.46	1.86	19	1
1:A:28:LEU:CD1	1:A:169:PHE:CZ	0.45	2.97	16	1
1:A:69:ILE:N	1:A:69:ILE:HD13	0.45	2.27	18	1
1:A:54:THR:O	1:A:54:THR:HG22	0.45	2.11	4	2
1:A:60:LEU:HD12	1:A:62:LEU:HD22	0.45	1.88	4	2
1:A:57:SER:CB	1:A:78:ILE:HG23	0.45	2.41	20	1
1:A:26:PRO:O	1:A:30:GLU:N	0.45	2.49	15	5
1:A:120:LEU:HD13	1:A:121:LYS:N	0.45	2.26	13	1
1:A:25:GLU:HB2	1:A:26:PRO:HD3	0.45	1.89	19	1
1:A:45:VAL:C	1:A:46:LEU:HD12	0.45	2.32	6	2
1:A:67:TYR:HA	1:A:156:ILE:HG23	0.45	1.88	4	4
1:A:43:LEU:HG	1:A:62:LEU:HD13	0.45	1.89	5	3
1:A:125:LYS:O	1:A:126:ALA:CB	0.45	2.64	11	1
1:A:27:VAL:HG22	1:A:33:LEU:HG	0.45	1.88	17	1
1:A:58:LEU:N	1:A:58:LEU:CD1	0.45	2.78	15	6
1:A:128:LEU:CD2	1:A:129:PHE:CD2	0.44	3.00	3	1
1:A:28:LEU:HD21	1:A:169:PHE:CE2	0.44	2.47	6	2
1:A:116:PHE:CD2	1:A:117:PHE:CE2	0.44	3.06	1	1
1:A:43:LEU:CD1	1:A:62:LEU:HD13	0.44	2.43	6	3
1:A:55:LEU:CD1	1:A:78:ILE:HD13	0.44	2.42	10	1
1:A:23:TRP:CE2	1:A:43:LEU:HD13	0.44	2.48	2	1
1:A:58:LEU:HB2	1:A:59:PRO:HD2	0.44	1.88	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ILE:HG21	1:A:169:PHE:CZ	0.44	2.48	2	1
1:A:28:LEU:HD13	1:A:168:ARG:HG3	0.44	1.90	9	1
1:A:159:LEU:HD11	1:A:165:TYR:CE1	0.44	2.47	13	1
1:A:48:ILE:C	1:A:50:PRO:HD3	0.44	2.33	17	1
1:A:89:VAL:HA	1:A:93:LEU:HD22	0.44	1.90	10	1
1:A:37:TYR:CD1	1:A:37:TYR:N	0.44	2.86	19	1
1:A:99:MET:CG	1:A:143:PHE:HB2	0.44	2.42	20	1
1:A:67:TYR:CE2	1:A:162:THR:HG22	0.44	2.47	3	1
1:A:94:LEU:HD22	1:A:98:ILE:CD1	0.44	2.43	14	1
1:A:55:LEU:HG	1:A:75:TYR:CE2	0.44	2.48	2	1
1:A:89:VAL:HG23	1:A:93:LEU:HB3	0.44	1.89	20	1
1:A:27:VAL:CG2	1:A:33:LEU:HD23	0.43	2.43	5	1
1:A:93:LEU:HD23	1:A:142:MET:CE	0.43	2.42	16	1
1:A:100:ILE:CG2	1:A:137:ILE:HG23	0.43	2.42	16	1
1:A:70:LEU:HD12	1:A:117:PHE:CE2	0.43	2.48	20	1
1:A:46:LEU:N	1:A:46:LEU:CD2	0.43	2.81	17	1
1:A:33:LEU:HD13	1:A:37:TYR:CB	0.43	2.42	9	1
1:A:43:LEU:CD2	1:A:62:LEU:HD11	0.43	2.41	9	1
1:A:28:LEU:HD11	1:A:165:TYR:CE2	0.43	2.48	8	1
1:A:63:CYS:SG	1:A:153:ALA:HB1	0.43	2.54	20	1
1:A:81:PHE:CE2	1:A:82:GLU:HG3	0.43	2.49	9	1
1:A:85:GLU:O	1:A:86:ARG:HG2	0.43	2.13	13	1
1:A:39:VAL:CG2	1:A:103:PHE:CZ	0.43	3.01	14	1
1:A:23:TRP:CZ3	1:A:41:LYS:CE	0.43	3.01	18	1
1:A:51:ARG:O	1:A:54:THR:HG22	0.43	2.14	2	1
1:A:81:PHE:CD2	1:A:140:PHE:CE1	0.43	3.06	6	3
1:A:53:ASN:O	1:A:54:THR:CG2	0.43	2.67	10	6
1:A:43:LEU:HG	1:A:62:LEU:HD12	0.43	1.89	4	2
1:A:133:LEU:HD11	1:A:169:PHE:CZ	0.43	2.49	16	2
1:A:28:LEU:HD21	1:A:165:TYR:HA	0.43	1.90	8	1
1:A:58:LEU:CB	1:A:59:PRO:CD	0.42	2.97	14	1
1:A:56:SER:CB	1:A:81:PHE:CE1	0.42	3.02	15	1
1:A:148:LEU:HD22	1:A:148:LEU:N	0.42	2.29	6	2
1:A:133:LEU:CD1	1:A:169:PHE:CE2	0.42	3.02	16	1
1:A:44:LYS:O	1:A:62:LEU:HB2	0.42	2.14	19	2
1:A:58:LEU:O	1:A:60:LEU:HD23	0.42	2.13	7	1
1:A:78:ILE:O	1:A:81:PHE:CD1	0.42	2.72	10	2
1:A:28:LEU:HD21	1:A:169:PHE:CZ	0.42	2.50	18	1
1:A:120:LEU:CD2	1:A:122:PHE:CZ	0.42	3.02	7	3
1:A:43:LEU:HD23	1:A:100:ILE:HD11	0.42	1.91	4	1
1:A:28:LEU:HD11	1:A:168:ARG:HB3	0.42	1.92	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TRP:NE1	1:A:43:LEU:HD13	0.42	2.29	9	1
1:A:160:TYR:O	1:A:166:ILE:HD11	0.42	2.15	14	3
1:A:57:SER:HB2	1:A:78:ILE:HD13	0.42	1.91	14	1
1:A:44:LYS:CD	1:A:150:LEU:HD12	0.42	2.44	19	1
1:A:59:PRO:CB	1:A:116:PHE:CE2	0.42	3.03	1	1
1:A:158:PHE:CG	1:A:160:TYR:CZ	0.42	3.07	3	1
1:A:81:PHE:CD2	1:A:82:GLU:N	0.42	2.88	8	1
1:A:44:LYS:HG2	1:A:150:LEU:HD13	0.42	1.91	10	1
1:A:27:VAL:HG23	1:A:33:LEU:CD2	0.42	2.42	15	1
1:A:93:LEU:H	1:A:93:LEU:CD1	0.42	2.27	16	1
1:A:46:LEU:HD12	1:A:46:LEU:N	0.42	2.29	6	2
1:A:27:VAL:CG2	1:A:33:LEU:CD1	0.42	2.98	19	1
1:A:89:VAL:HG22	1:A:94:LEU:CG	0.42	2.44	2	1
1:A:105:ILE:HD13	1:A:135:LEU:HD13	0.42	1.92	16	1
1:A:68:LYS:O	1:A:159:LEU:CD1	0.42	2.68	1	1
1:A:43:LEU:CG	1:A:62:LEU:HD13	0.42	2.45	7	5
1:A:133:LEU:CD1	1:A:169:PHE:CZ	0.42	3.03	16	1
1:A:93:LEU:HD12	1:A:93:LEU:N	0.41	2.30	4	2
1:A:148:LEU:C	1:A:149:ILE:HD12	0.41	2.35	9	2
1:A:108:TYR:CD2	1:A:112:GLN:HB3	0.41	2.50	1	1
1:A:128:LEU:H	1:A:128:LEU:HD22	0.41	1.75	13	1
1:A:85:GLU:HG2	1:A:93:LEU:HD11	0.41	1.93	7	1
1:A:52:SER:O	1:A:54:THR:HG23	0.41	2.15	8	1
1:A:81:PHE:CE2	1:A:89:VAL:CG1	0.41	3.03	10	1
1:A:81:PHE:CZ	1:A:89:VAL:HG12	0.41	2.50	11	2
1:A:110:ASP:O	1:A:113:VAL:HG22	0.41	2.15	5	1
1:A:46:LEU:HD21	1:A:150:LEU:HB3	0.41	1.92	6	2
1:A:166:ILE:HG23	1:A:170:ILE:CG1	0.41	2.43	6	2
1:A:93:LEU:N	1:A:93:LEU:HD12	0.41	2.31	10	1
1:A:39:VAL:CG2	1:A:103:PHE:CE2	0.41	3.03	14	1
1:A:105:ILE:HG23	1:A:133:LEU:HG	0.41	1.92	2	1
1:A:28:LEU:HD23	1:A:168:ARG:CG	0.41	2.45	3	1
1:A:57:SER:CB	1:A:78:ILE:HG12	0.41	2.45	16	1
1:A:37:TYR:CE2	1:A:103:PHE:CE1	0.41	3.09	19	1
1:A:64:ASP:OD1	1:A:69:ILE:HD12	0.41	2.15	1	1
1:A:54:THR:HG22	1:A:55:LEU:H	0.41	1.76	5	1
1:A:64:ASP:N	1:A:67:TYR:O	0.41	2.52	5	1
1:A:47:ARG:O	1:A:60:LEU:HB2	0.41	2.16	7	1
1:A:23:TRP:O	1:A:27:VAL:CG1	0.41	2.69	9	1
1:A:88:ARG:HB3	1:A:91:GLN:HG2	0.41	1.93	10	1
1:A:89:VAL:C	1:A:93:LEU:HD11	0.41	2.36	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:GLU:CB	1:A:26:PRO:CD	0.41	2.99	8	1
1:A:133:LEU:HD13	1:A:165:TYR:CE1	0.41	2.51	9	1
1:A:93:LEU:C	1:A:93:LEU:CD2	0.41	2.89	16	1
1:A:68:LYS:CE	1:A:158:PHE:CE1	0.41	3.04	20	1
1:A:81:PHE:CE2	1:A:89:VAL:HG23	0.40	2.51	16	1
1:A:167:ALA:HA	1:A:171:GLU:CB	0.40	2.47	2	1
1:A:24:LEU:O	1:A:28:LEU:HD13	0.40	2.17	8	1
1:A:27:VAL:HG13	1:A:28:LEU:N	0.40	2.31	11	1
1:A:68:LYS:HG3	1:A:156:ILE:HG21	0.40	1.92	14	1
1:A:128:LEU:H	1:A:128:LEU:HD23	0.40	1.76	10	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/178 (84%)	137±2 (92±2%)	9±2 (6±1%)	3±1 (2±1%)	8	47
All	All	3000/3560 (84%)	2746 (92%)	188 (6%)	66 (2%)	8	47

All 12 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	119	GLY	20
1	A	91	GLN	14
1	A	126	ALA	11
1	A	96	SER	7
1	A	84	LYS	4
1	A	33	LEU	2
1	A	64	ASP	2
1	A	57	SER	2
1	A	161	GLY	1
1	A	162	THR	1
1	A	128	LEU	1
1	A	59	PRO	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	133/155 (86%)	115±3 (87±2%)	18±3 (13±2%)	6	46
All	All	2660/3100 (86%)	2308 (87%)	352 (13%)	6	46

All 69 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	69	ILE	20
1	A	114	GLN	19
1	A	76	LYS	16
1	A	128	LEU	16
1	A	58	LEU	15
1	A	159	LEU	13
1	A	168	ARG	13
1	A	133	LEU	11
1	A	25	GLU	11
1	A	138	ASN	10
1	A	70	LEU	9
1	A	95	ASN	9
1	A	142	MET	9
1	A	81	PHE	9
1	A	116	PHE	9
1	A	83	ARG	8
1	A	23	TRP	8
1	A	124	GLN	8
1	A	49	TYR	8
1	A	33	LEU	8
1	A	64	ASP	7
1	A	117	PHE	7
1	A	55	LEU	6
1	A	99	MET	6
1	A	86	ARG	5
1	A	62	LEU	5
1	A	97	GLU	5
1	A	92	ASN	4
1	A	102	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	120	LEU	4
1	A	48	ILE	4
1	A	38	LYS	4
1	A	145	ARG	3
1	A	68	LYS	3
1	A	164	ARG	3
1	A	165	TYR	3
1	A	160	TYR	3
1	A	29	CYS	3
1	A	36	ASN	3
1	A	41	LYS	3
1	A	28	LEU	2
1	A	91	GLN	2
1	A	88	ARG	2
1	A	144	ASN	2
1	A	35	HIS	2
1	A	146	ASP	2
1	A	74	ASN	2
1	A	56	SER	2
1	A	150	LEU	2
1	A	84	LYS	1
1	A	46	LEU	1
1	A	47	ARG	1
1	A	125	LYS	1
1	A	44	LYS	1
1	A	121	LYS	1
1	A	37	TYR	1
1	A	51	ARG	1
1	A	57	SER	1
1	A	123	LYS	1
1	A	171	GLU	1
1	A	54	THR	1
1	A	143	PHE	1
1	A	158	PHE	1
1	A	93	LEU	1
1	A	90	THR	1
1	A	96	SER	1
1	A	139	ASP	1
1	A	106	ARG	1
1	A	112	GLN	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.



## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 79% 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	1997
Number of shifts mapped to atoms	1997
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	176	$-0.18 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	167	$-0.01 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	168	$0.13 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	168	$0.42 \pm 0.46$	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 80%, i.e. 1731 atoms were assigned a chemical shift out of a possible 2175. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	735/747 (98%)	297/302 (98%)	293/300 (98%)	145/145 (100%)
Sidechain	914/1208 (76%)	615/785 (78%)	285/368 (77%)	14/55 (25%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	82/220 (37%)	79/106 (75%)	2/109 (2%)	1/5 (20%)
Overall	1731/2175 (80%)	991/1193 (83%)	580/777 (75%)	160/205 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1997 atoms were assigned a chemical shift out of a possible 2518. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	859/885 (97%)	347/358 (97%)	344/356 (97%)	168/171 (98%)
Sidechain	1046/1387 (75%)	704/901 (78%)	328/424 (77%)	14/62 (23%)
Aromatic	92/246 (37%)	87/119 (73%)	4/118 (3%)	1/9 (11%)
Overall	1997/2518 (79%)	1138/1378 (83%)	676/898 (75%)	183/242 (76%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

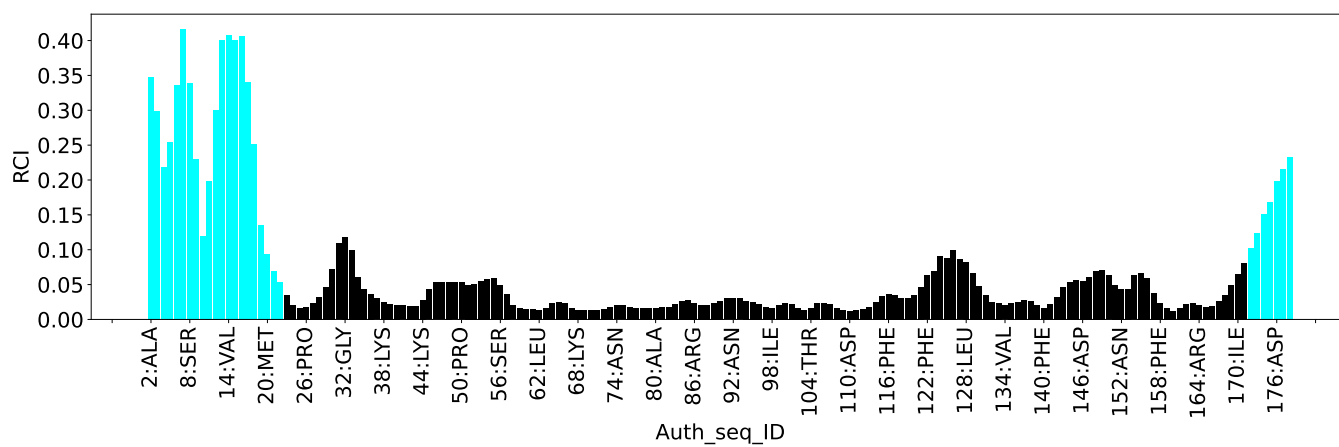
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	68	LYS	HE3	1.35	1.92 – 3.89	-7.9
1	A	41	LYS	HG3	-0.50	0.04 – 2.67	-7.0
1	A	41	LYS	HD3	0.13	0.54 – 2.65	-7.0
1	A	41	LYS	HB3	0.37	0.46 – 3.04	-5.4
1	A	68	LYS	HD2	0.54	0.58 – 2.64	-5.2

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

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	2262
Intra-residue ( $ i-j =0$ )	1041
Sequential ( $ i-j =1$ )	568
Medium range ( $ i-j >1$ and $ i-j <5$ )	210
Long range ( $ i-j \geq 5$ )	443
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	228
Number of unmapped restraints	0
Number of restraints per residue	14.0
Number of long range restraints per residue <sup>1</sup>	2.5

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	65.5	0.2
0.2-0.5 (Medium)	27.2	0.5
>0.5 (Large)	None	None

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	3.6	4.78
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

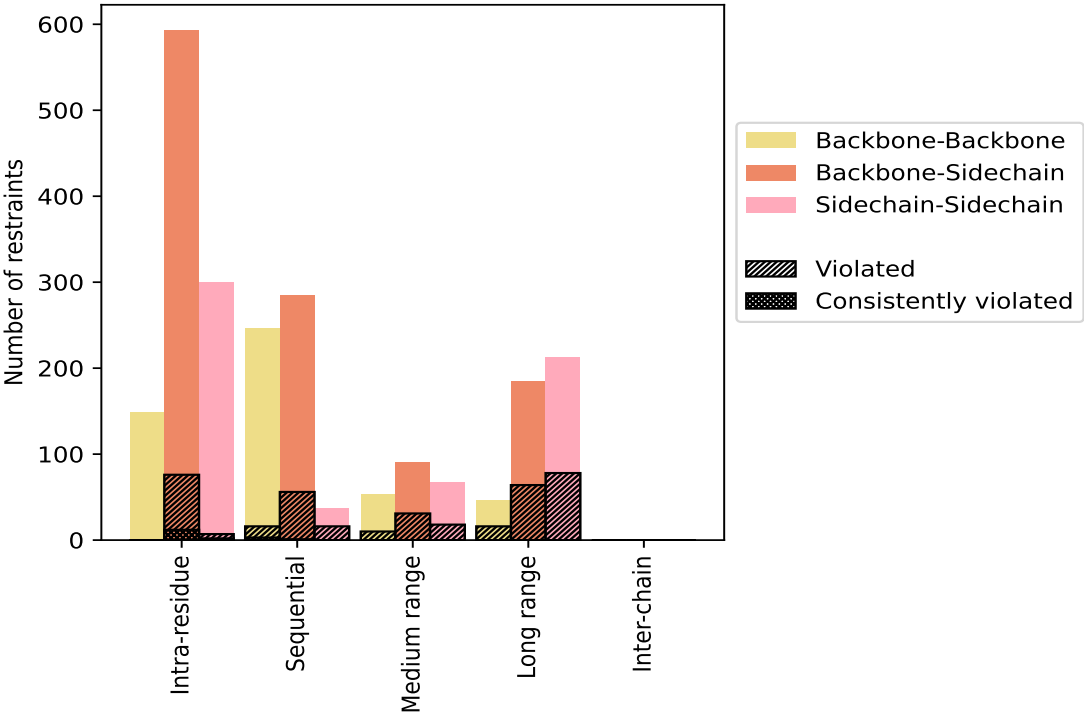
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">1041</a>	<a href="#">46.0</a>	<a href="#">83</a>	<a href="#">8.0</a>	<a href="#">3.7</a>	<a href="#">14</a>	<a href="#">1.3</a>	<a href="#">0.6</a>
Backbone-Backbone	148	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	593	26.2	76	12.8	3.4	12	2.0	0.5
Sidechain-Sidechain	300	13.3	7	2.3	0.3	2	0.7	0.1
<a href="#">Sequential ( i-j =1)</a>	<a href="#">568</a>	<a href="#">25.1</a>	<a href="#">88</a>	<a href="#">15.5</a>	<a href="#">3.9</a>	<a href="#">4</a>	<a href="#">0.7</a>	<a href="#">0.2</a>
Backbone-Backbone	246	10.9	16	6.5	0.7	3	1.2	0.1
Backbone-Sidechain	285	12.6	56	19.6	2.5	1	0.4	0.0
Sidechain-Sidechain	37	1.6	16	43.2	0.7	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">210</a>	<a href="#">9.3</a>	<a href="#">59</a>	<a href="#">28.1</a>	<a href="#">2.6</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	53	2.3	10	18.9	0.4	0	0.0	0.0
Backbone-Sidechain	90	4.0	31	34.4	1.4	0	0.0	0.0
Sidechain-Sidechain	67	3.0	18	26.9	0.8	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">443</a>	<a href="#">19.6</a>	<a href="#">158</a>	<a href="#">35.7</a>	<a href="#">7.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	46	2.0	16	34.8	0.7	0	0.0	0.0
Backbone-Sidechain	185	8.2	64	34.6	2.8	0	0.0	0.0
Sidechain-Sidechain	212	9.4	78	36.8	3.4	0	0.0	0.0
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">2262</a>	<a href="#">100.0</a>	<a href="#">388</a>	<a href="#">17.2</a>	<a href="#">17.2</a>	<a href="#">18</a>	<a href="#">0.8</a>	<a href="#">0.8</a>
Backbone-Backbone	493	21.8	42	8.5	1.9	3	0.6	0.1
Backbone-Sidechain	1153	51.0	227	19.7	10.0	13	1.1	0.6
Sidechain-Sidechain	616	27.2	119	19.3	5.3	2	0.3	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	25	22	11	33	0	91	0.17	0.48	0.07	0.16
2	33	19	14	33	0	99	0.19	0.48	0.08	0.17
3	26	24	7	32	0	89	0.17	0.36	0.06	0.16
4	29	21	14	38	0	102	0.18	0.47	0.06	0.16
5	31	24	17	41	0	113	0.17	0.43	0.06	0.15
6	32	23	8	26	0	89	0.17	0.48	0.06	0.15
7	27	19	14	24	0	84	0.18	0.44	0.07	0.16
8	29	21	9	30	0	89	0.17	0.48	0.06	0.14
9	29	24	14	41	0	108	0.18	0.4	0.07	0.15
10	32	27	16	32	0	107	0.16	0.41	0.06	0.15

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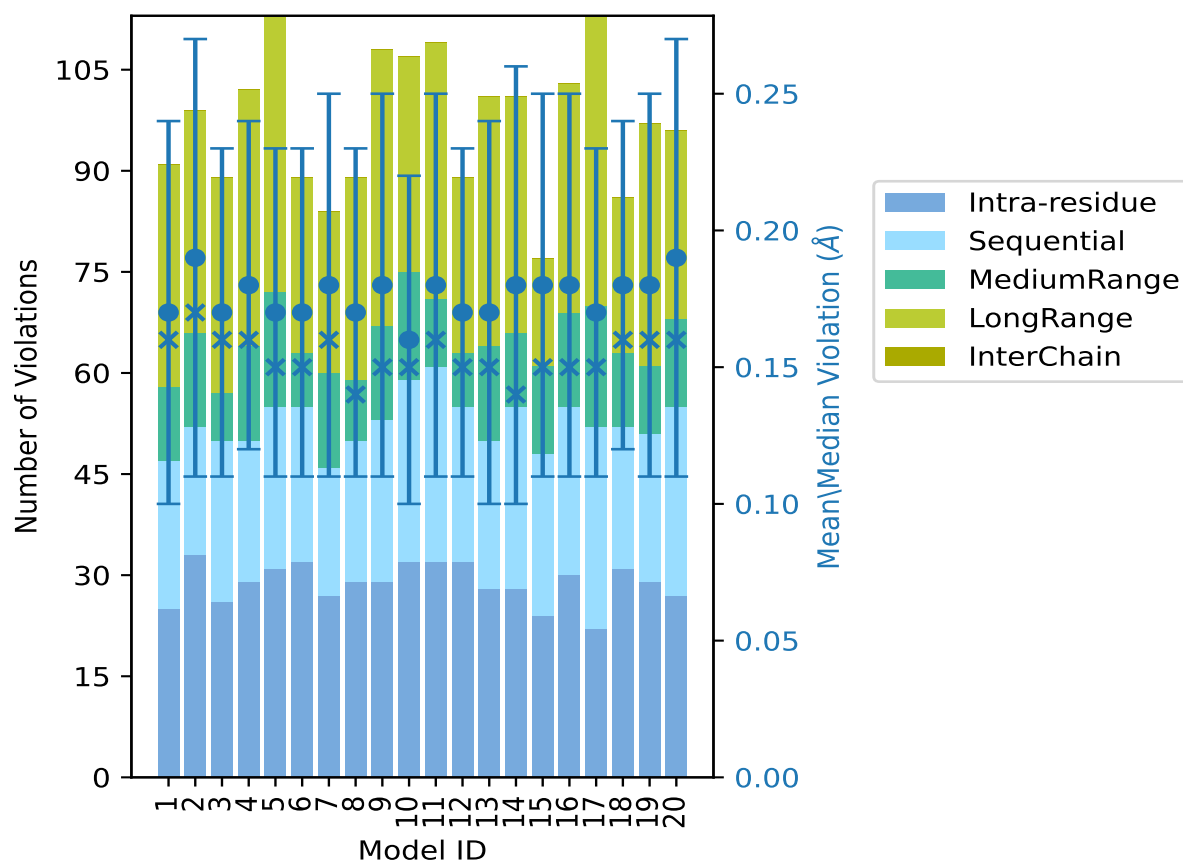
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	32	29	10	38	0	109	0.18	0.47	0.07	0.16
12	32	23	8	26	0	89	0.17	0.48	0.06	0.15
13	28	22	14	37	0	101	0.17	0.39	0.07	0.15
14	28	27	11	35	0	101	0.18	0.47	0.08	0.14
15	24	24	13	16	0	77	0.18	0.48	0.07	0.15
16	30	25	14	34	0	103	0.18	0.49	0.07	0.15
17	22	30	18	43	0	113	0.17	0.43	0.06	0.15
18	31	21	11	23	0	86	0.18	0.5	0.06	0.16
19	29	22	10	36	0	97	0.18	0.39	0.07	0.16
20	27	28	13	28	0	96	0.19	0.49	0.08	0.16

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

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

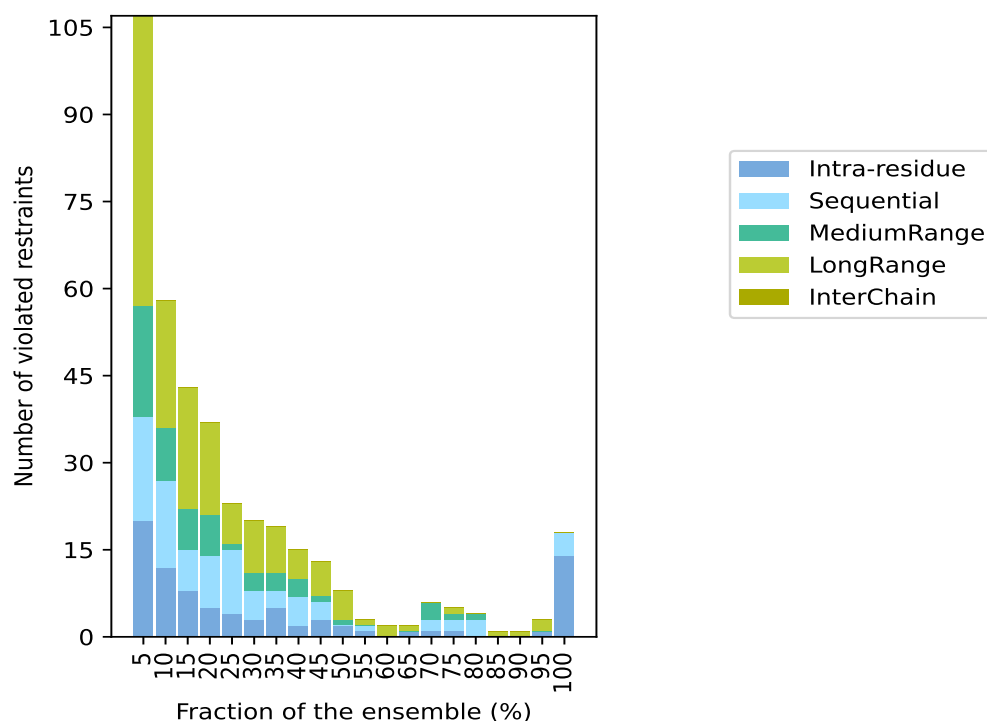
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1874(IR:958, SQ:480, MR:151, LR:285, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
20	18	19	50	0	107	1	5.0
12	15	9	22	0	58	2	10.0
8	7	7	21	0	43	3	15.0
5	9	7	16	0	37	4	20.0
4	11	1	7	0	23	5	25.0
3	5	3	9	0	20	6	30.0
5	3	3	8	0	19	7	35.0
2	5	3	5	0	15	8	40.0
3	3	1	6	0	13	9	45.0
2	0	1	5	0	8	10	50.0
1	1	0	1	0	3	11	55.0
0	0	0	2	0	2	12	60.0
1	0	0	1	0	2	13	65.0
1	2	3	0	0	6	14	70.0
1	2	1	1	0	5	15	75.0
0	3	1	0	0	4	16	80.0
0	0	0	1	0	1	17	85.0
0	0	0	1	0	1	18	90.0
1	0	0	2	0	3	19	95.0
14	4	0	0	0	18	20	100.0

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

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

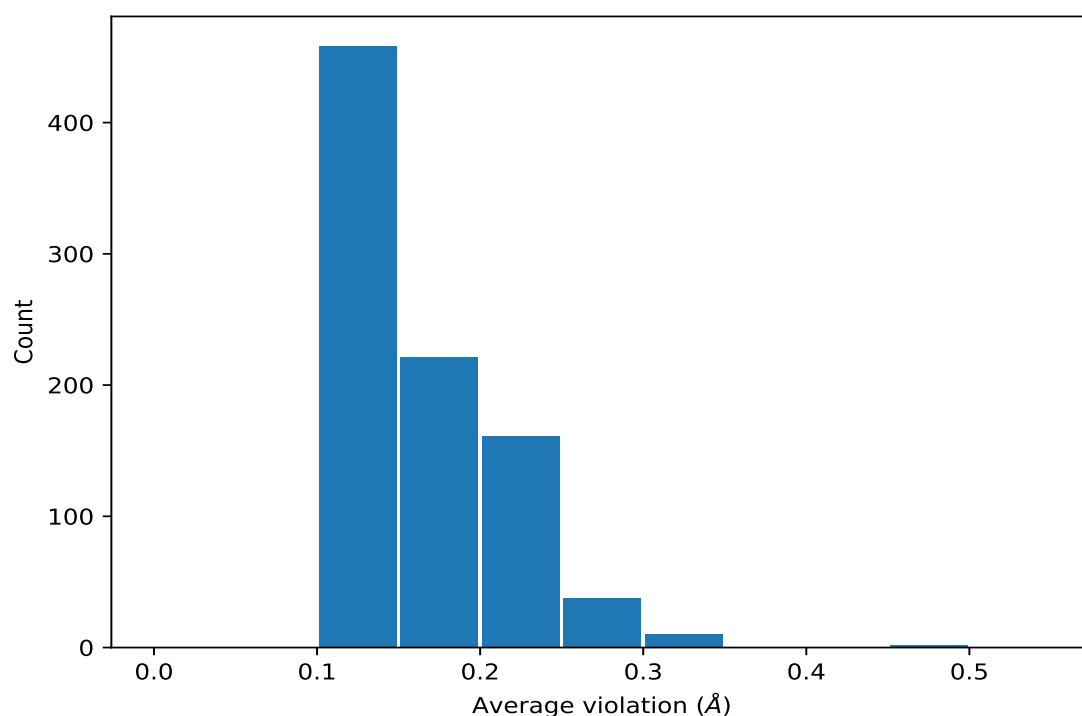
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	20	0.28	0.02	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	20	0.28	0.02	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	20	0.28	0.02	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	20	0.28	0.01	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	20	0.28	0.01	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	20	0.28	0.01	0.28
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	20	0.28	0.01	0.28
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	20	0.28	0.01	0.28
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	20	0.28	0.01	0.28
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	20	0.26	0.02	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	20	0.26	0.02	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	20	0.26	0.02	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	20	0.26	0.0	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	20	0.26	0.0	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	20	0.26	0.0	0.26
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	20	0.25	0.01	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	20	0.25	0.01	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	20	0.25	0.01	0.25
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	20	0.22	0.0	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	20	0.22	0.0	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	20	0.22	0.0	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	20	0.22	0.04	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	20	0.22	0.04	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	20	0.22	0.04	0.2
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	20	0.21	0.0	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	20	0.21	0.0	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	20	0.21	0.0	0.21
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	20	0.2	0.01	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	20	0.2	0.01	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	20	0.2	0.01	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	20	0.2	0.01	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	20	0.2	0.01	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	20	0.2	0.01	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	20	0.19	0.01	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	20	0.19	0.01	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	20	0.19	0.01	0.19
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	20	0.16	0.02	0.16
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	20	0.15	0.03	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	20	0.14	0.02	0.14
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	20	0.14	0.01	0.14
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	20	0.14	0.01	0.14
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	20	0.12	0.01	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	20	0.12	0.01	0.12
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	19	0.21	0.05	0.21
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	19	0.21	0.05	0.21
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	19	0.19	0.04	0.18
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	19	0.19	0.04	0.18
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	19	0.19	0.04	0.18
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	19	0.17	0.04	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	19	0.17	0.04	0.16
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	18	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	18	0.14	0.03	0.14
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	18	0.14	0.03	0.14
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	18	0.14	0.03	0.14
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	18	0.14	0.03	0.14
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	18	0.14	0.03	0.14
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	18	0.14	0.03	0.14
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	18	0.14	0.03	0.14
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	18	0.14	0.03	0.14
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	17	0.19	0.06	0.19
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	17	0.19	0.06	0.19
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	16	0.21	0.1	0.18
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	16	0.21	0.1	0.18
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	16	0.21	0.1	0.18
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	16	0.19	0.05	0.18
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	16	0.16	0.04	0.16
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	16	0.16	0.04	0.16
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	16	0.16	0.04	0.16
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	16	0.12	0.01	0.12
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	15	0.21	0.06	0.2
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	15	0.21	0.06	0.2
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	15	0.21	0.06	0.2
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	15	0.19	0.07	0.16
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	15	0.19	0.07	0.16
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	15	0.19	0.07	0.16
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	15	0.17	0.04	0.19
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	15	0.17	0.04	0.19
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	15	0.16	0.05	0.14
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	15	0.16	0.04	0.15
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	14	0.23	0.08	0.22
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	14	0.23	0.08	0.22
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	14	0.23	0.08	0.22
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	14	0.18	0.05	0.17
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	14	0.18	0.05	0.17
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	14	0.14	0.02	0.14
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	14	0.14	0.02	0.14
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	14	0.14	0.02	0.14
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	14	0.13	0.03	0.12
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	14	0.13	0.02	0.13
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	14	0.12	0.01	0.12
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	13	0.22	0.07	0.21
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	13	0.22	0.07	0.21
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	13	0.22	0.07	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	13	0.22	0.07	0.21
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	13	0.22	0.07	0.21
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	13	0.22	0.07	0.21
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	13	0.22	0.02	0.22
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	13	0.22	0.02	0.22
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	13	0.22	0.02	0.22
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	12	0.22	0.08	0.22
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	12	0.22	0.08	0.22
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	12	0.22	0.08	0.22
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	12	0.15	0.04	0.12
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	12	0.15	0.04	0.12
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	12	0.15	0.04	0.12
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	11	0.21	0.03	0.22
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	11	0.21	0.03	0.22
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	11	0.21	0.03	0.22
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	11	0.18	0.04	0.17
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	11	0.18	0.04	0.17
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	11	0.18	0.04	0.17
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	11	0.15	0.03	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	11	0.15	0.03	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	11	0.15	0.03	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	11	0.15	0.03	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	11	0.15	0.03	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	11	0.15	0.03	0.14
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	10	0.27	0.07	0.25
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	10	0.27	0.07	0.25
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	10	0.27	0.07	0.25
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	10	0.23	0.07	0.22
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	10	0.23	0.07	0.22
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	10	0.23	0.07	0.22
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	10	0.23	0.07	0.22
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	10	0.23	0.07	0.22
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	10	0.23	0.07	0.22
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	10	0.21	0.11	0.19
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	10	0.21	0.11	0.19
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	10	0.18	0.04	0.18
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	10	0.18	0.04	0.18
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	10	0.18	0.04	0.18
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	10	0.14	0.04	0.15
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	10	0.14	0.04	0.15
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	10	0.14	0.04	0.15
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	10	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	10	0.14	0.04	0.12
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	10	0.14	0.04	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	10	0.12	0.02	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	10	0.12	0.02	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	10	0.12	0.02	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	10	0.12	0.02	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	10	0.12	0.02	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	10	0.12	0.02	0.12
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	10	0.12	0.01	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	10	0.12	0.01	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	10	0.12	0.01	0.11
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	9	0.23	0.0	0.23
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	9	0.23	0.0	0.23
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	9	0.23	0.0	0.23
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	9	0.21	0.1	0.17
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	9	0.21	0.1	0.17
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	9	0.21	0.1	0.17
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	9	0.2	0.05	0.2
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	9	0.2	0.05	0.2
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	9	0.2	0.05	0.2
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	9	0.18	0.05	0.17
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	9	0.18	0.05	0.17
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	9	0.18	0.05	0.17
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	9	0.17	0.03	0.17
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	9	0.17	0.03	0.17
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	9	0.17	0.03	0.17
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	9	0.17	0.06	0.16
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	9	0.17	0.06	0.16
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	9	0.17	0.06	0.16
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	9	0.17	0.06	0.16
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	9	0.17	0.06	0.16
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	9	0.17	0.06	0.16
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	9	0.16	0.05	0.16
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	9	0.16	0.05	0.16
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	9	0.16	0.05	0.16
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	9	0.16	0.04	0.16
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	9	0.16	0.04	0.16
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	9	0.16	0.04	0.16
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	9	0.16	0.04	0.16
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	9	0.16	0.04	0.16
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	9	0.16	0.04	0.16
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	9	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	9	0.16	0.04	0.16
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	9	0.16	0.04	0.16
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	9	0.14	0.03	0.13
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	9	0.14	0.03	0.13
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	9	0.14	0.03	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	9	0.14	0.01	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	9	0.14	0.01	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	9	0.14	0.01	0.13
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	9	0.13	0.02	0.13
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	9	0.13	0.02	0.13
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	9	0.13	0.02	0.13
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	9	0.13	0.02	0.13
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	9	0.11	0.01	0.11
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	8	0.22	0.01	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	8	0.22	0.01	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	8	0.22	0.01	0.23
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	8	0.22	0.03	0.21
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	8	0.22	0.03	0.21
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	8	0.2	0.05	0.18
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	8	0.2	0.05	0.18
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	8	0.2	0.05	0.22
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	8	0.2	0.05	0.22
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	8	0.18	0.09	0.15
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	8	0.18	0.09	0.15
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	8	0.18	0.09	0.15
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	8	0.17	0.06	0.13
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	8	0.17	0.06	0.13
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	8	0.15	0.04	0.13
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	8	0.15	0.04	0.13
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	8	0.15	0.04	0.13
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	8	0.14	0.02	0.15
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	8	0.14	0.03	0.13
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	8	0.14	0.03	0.13
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	8	0.14	0.02	0.14
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	8	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	8	0.14	0.02	0.14
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	8	0.14	0.02	0.14
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	8	0.14	0.02	0.14
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	8	0.14	0.02	0.14
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	8	0.14	0.03	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	8	0.14	0.03	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	8	0.14	0.03	0.12
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	8	0.14	0.02	0.13
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	8	0.14	0.02	0.13
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	8	0.14	0.02	0.13
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	8	0.14	0.02	0.13
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	8	0.14	0.02	0.13
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	8	0.14	0.02	0.13
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	8	0.14	0.03	0.13
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	8	0.14	0.03	0.13
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	8	0.14	0.03	0.13
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	8	0.13	0.02	0.12
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	8	0.13	0.02	0.12
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	8	0.13	0.02	0.12
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	8	0.12	0.02	0.12
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	8	0.12	0.02	0.12
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	8	0.12	0.02	0.12
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	7	0.48	0.0	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	7	0.48	0.0	0.48
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	7	0.24	0.08	0.26
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	7	0.24	0.08	0.26
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	7	0.24	0.04	0.24
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	7	0.24	0.04	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	7	0.24	0.04	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	7	0.24	0.04	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	7	0.24	0.04	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	7	0.24	0.04	0.24
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	7	0.21	0.0	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	7	0.21	0.0	0.21
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	7	0.21	0.1	0.18
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	7	0.18	0.04	0.16
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	7	0.18	0.04	0.16
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	7	0.18	0.04	0.16
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	7	0.18	0.04	0.16
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	7	0.18	0.04	0.16
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	7	0.18	0.04	0.16
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	7	0.18	0.09	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	7	0.18	0.09	0.14
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	7	0.18	0.09	0.14
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	7	0.18	0.05	0.17
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	7	0.17	0.04	0.18
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	7	0.17	0.04	0.18
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	7	0.17	0.04	0.18
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	7	0.17	0.06	0.15
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	7	0.17	0.06	0.15
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	7	0.17	0.06	0.15
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	7	0.14	0.02	0.15
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	7	0.14	0.02	0.15
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	7	0.14	0.02	0.15
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	7	0.14	0.03	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	7	0.14	0.03	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	7	0.14	0.03	0.13
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	7	0.13	0.03	0.13
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	7	0.13	0.03	0.13
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	7	0.13	0.03	0.13
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	7	0.13	0.03	0.12
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	7	0.13	0.03	0.12
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	7	0.13	0.03	0.11
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	7	0.13	0.03	0.11
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	7	0.13	0.03	0.11
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	7	0.13	0.03	0.11
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	7	0.13	0.03	0.11
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	7	0.13	0.03	0.11
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	7	0.12	0.02	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	7	0.12	0.02	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	7	0.12	0.02	0.12
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	7	0.12	0.02	0.11
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	7	0.12	0.02	0.11
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	7	0.12	0.02	0.11
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	7	0.12	0.02	0.1
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	7	0.12	0.01	0.11
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD21	6	0.26	0.07	0.3
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD22	6	0.26	0.07	0.3
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD23	6	0.26	0.07	0.3
(1,700)	1:55:A:LEU:HD11	1:55:A:LEU:H	6	0.22	0.05	0.2
(1,700)	1:55:A:LEU:HD12	1:55:A:LEU:H	6	0.22	0.05	0.2
(1,700)	1:55:A:LEU:HD13	1:55:A:LEU:H	6	0.22	0.05	0.2
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD21	6	0.22	0.05	0.24
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD22	6	0.22	0.05	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD23	6	0.22	0.05	0.24
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB2	6	0.22	0.09	0.2
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB3	6	0.22	0.09	0.2
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB2	6	0.22	0.09	0.2
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB3	6	0.22	0.09	0.2
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB2	6	0.22	0.09	0.2
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB3	6	0.22	0.09	0.2
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD1	6	0.21	0.09	0.19
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD2	6	0.21	0.09	0.19
(1,409)	1:171:A:GLU:HB2	1:172:A:GLN:H	6	0.21	0.05	0.2
(1,409)	1:171:A:GLU:HB3	1:172:A:GLN:H	6	0.21	0.05	0.2
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG2	6	0.18	0.06	0.18
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG3	6	0.18	0.06	0.18
(1,183)	1:135:A:LEU:HD21	1:23:A:TRP:HH2	6	0.17	0.03	0.16
(1,183)	1:135:A:LEU:HD22	1:23:A:TRP:HH2	6	0.17	0.03	0.16
(1,183)	1:135:A:LEU:HD23	1:23:A:TRP:HH2	6	0.17	0.03	0.16
(1,298)	1:24:A:LEU:HD11	1:69:A:ILE:H	6	0.16	0.02	0.16
(1,298)	1:24:A:LEU:HD12	1:69:A:ILE:H	6	0.16	0.02	0.16
(1,298)	1:24:A:LEU:HD13	1:69:A:ILE:H	6	0.16	0.02	0.16
(1,13)	1:142:A:MET:HE1	1:94:A:LEU:HG	6	0.16	0.04	0.16
(1,13)	1:142:A:MET:HE2	1:94:A:LEU:HG	6	0.16	0.04	0.16
(1,13)	1:142:A:MET:HE3	1:94:A:LEU:HG	6	0.16	0.04	0.16
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB2	6	0.15	0.04	0.14
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB3	6	0.15	0.04	0.14
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG21	6	0.15	0.05	0.12
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG22	6	0.15	0.05	0.12
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG23	6	0.15	0.05	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG21	6	0.15	0.05	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG22	6	0.15	0.05	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG23	6	0.15	0.05	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD11	6	0.15	0.04	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD12	6	0.15	0.04	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD13	6	0.15	0.04	0.12
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB1	6	0.14	0.03	0.14
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB2	6	0.14	0.03	0.14
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB3	6	0.14	0.03	0.14
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD11	6	0.14	0.02	0.13
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD12	6	0.14	0.02	0.13
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD13	6	0.14	0.02	0.13
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG12	6	0.13	0.02	0.12
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG13	6	0.13	0.02	0.12
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG12	6	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG13	6	0.13	0.02	0.12
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG11	6	0.13	0.01	0.12
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG12	6	0.13	0.01	0.12
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG13	6	0.13	0.01	0.12
(1,951)	1:89:A:VAL:HG21	1:140:A:PHE:HZ	6	0.12	0.02	0.12
(1,951)	1:89:A:VAL:HG22	1:140:A:PHE:HZ	6	0.12	0.02	0.12
(1,951)	1:89:A:VAL:HG23	1:140:A:PHE:HZ	6	0.12	0.02	0.12
(1,1759)	1:54:A:THR:HB	1:55:A:LEU:H	6	0.12	0.01	0.12
(1,748)	1:62:A:LEU:HD11	1:45:A:VAL:HA	6	0.12	0.03	0.11
(1,748)	1:62:A:LEU:HD12	1:45:A:VAL:HA	6	0.12	0.03	0.11
(1,748)	1:62:A:LEU:HD13	1:45:A:VAL:HA	6	0.12	0.03	0.11
(1,958)	1:90:A:THR:HB	1:91:A:GLN:H	5	0.33	0.06	0.35
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG21	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG22	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG23	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG21	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG22	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG23	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG21	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG22	5	0.2	0.04	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG23	5	0.2	0.04	0.22
(1,302)	1:15:A:THR:HG21	1:15:A:THR:HA	5	0.2	0.03	0.21
(1,302)	1:15:A:THR:HG22	1:15:A:THR:HA	5	0.2	0.03	0.21
(1,302)	1:15:A:THR:HG23	1:15:A:THR:HA	5	0.2	0.03	0.21
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD11	5	0.19	0.06	0.16
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD12	5	0.19	0.06	0.16
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD13	5	0.19	0.06	0.16
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB2	5	0.18	0.05	0.18
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB3	5	0.18	0.05	0.18
(1,573)	1:33:A:LEU:HD11	1:33:A:LEU:H	5	0.16	0.03	0.14
(1,573)	1:33:A:LEU:HD12	1:33:A:LEU:H	5	0.16	0.03	0.14
(1,573)	1:33:A:LEU:HD13	1:33:A:LEU:H	5	0.16	0.03	0.14
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB2	5	0.15	0.04	0.13
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB3	5	0.15	0.04	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB2	5	0.15	0.04	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB3	5	0.15	0.04	0.13
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE1	5	0.15	0.03	0.15
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE2	5	0.15	0.03	0.15
(1,1423)	1:170:A:ILE:HG21	1:171:A:GLU:HA	5	0.14	0.01	0.14
(1,1423)	1:170:A:ILE:HG22	1:171:A:GLU:HA	5	0.14	0.01	0.14
(1,1423)	1:170:A:ILE:HG23	1:171:A:GLU:HA	5	0.14	0.01	0.14
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB2	5	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB3	5	0.14	0.02	0.14
(1,669)	1:47:A:ARG:HD2	1:48:A:ILE:H	5	0.14	0.04	0.11
(1,669)	1:47:A:ARG:HD3	1:48:A:ILE:H	5	0.14	0.04	0.11
(1,1681)	1:170:A:ILE:H	1:167:A:ALA:HA	5	0.14	0.02	0.14
(1,1018)	1:99:A:MET:HG2	1:100:A:ILE:H	5	0.13	0.02	0.12
(1,1018)	1:99:A:MET:HG3	1:100:A:ILE:H	5	0.13	0.02	0.12
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG2	5	0.13	0.02	0.13
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG3	5	0.13	0.02	0.13
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD1	5	0.13	0.02	0.14
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD2	5	0.13	0.02	0.14
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD1	5	0.13	0.02	0.14
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD2	5	0.13	0.02	0.14
(1,1012)	1:99:A:MET:HE1	1:99:A:MET:HA	5	0.13	0.02	0.12
(1,1012)	1:99:A:MET:HE2	1:99:A:MET:HA	5	0.13	0.02	0.12
(1,1012)	1:99:A:MET:HE3	1:99:A:MET:HA	5	0.13	0.02	0.12
(1,1159)	1:109:A:ASN:HB2	1:130:A:PRO:HA	5	0.13	0.02	0.12
(1,1159)	1:109:A:ASN:HB3	1:130:A:PRO:HA	5	0.13	0.02	0.12
(1,1266)	1:142:A:MET:HE1	1:97:A:GLU:H	5	0.13	0.03	0.13
(1,1266)	1:142:A:MET:HE2	1:97:A:GLU:H	5	0.13	0.03	0.13
(1,1266)	1:142:A:MET:HE3	1:97:A:GLU:H	5	0.13	0.03	0.13
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG21	5	0.13	0.03	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG22	5	0.13	0.03	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG23	5	0.13	0.03	0.11
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE1	5	0.12	0.01	0.13
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE2	5	0.12	0.01	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE1	5	0.12	0.01	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE2	5	0.12	0.01	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE1	5	0.12	0.01	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE2	5	0.12	0.01	0.13
(1,1596)	1:102:A:SER:H	1:101:A:HIS:HD2	5	0.12	0.03	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD1	5	0.12	0.02	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD2	5	0.12	0.02	0.11
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD1	5	0.12	0.02	0.11
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD2	5	0.12	0.02	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD1	5	0.12	0.02	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD2	5	0.12	0.02	0.11
(1,1854)	1:146:A:ASP:H	1:147:A:GLN:H	5	0.11	0.01	0.11
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD1	4	0.35	0.12	0.41
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD2	4	0.35	0.12	0.41
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD1	4	0.35	0.12	0.41
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD2	4	0.35	0.12	0.41
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD1	4	0.35	0.12	0.41

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD2	4	0.35	0.12	0.41
(1,578)	1:34:A:GLY:HA2	1:36:A:ASN:H	4	0.29	0.12	0.22
(1,578)	1:34:A:GLY:HA3	1:36:A:ASN:H	4	0.29	0.12	0.22
(1,963)	1:92:A:ASN:HA	1:92:A:ASN:HD22	4	0.29	0.01	0.29
(1,678)	1:48:A:ILE:HD11	1:48:A:ILE:H	4	0.27	0.05	0.26
(1,678)	1:48:A:ILE:HD12	1:48:A:ILE:H	4	0.27	0.05	0.26
(1,678)	1:48:A:ILE:HD13	1:48:A:ILE:H	4	0.27	0.05	0.26
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB2	4	0.23	0.04	0.24
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB3	4	0.23	0.04	0.24
(1,425)	1:62:A:LEU:HD11	1:43:A:LEU:HA	4	0.21	0.05	0.2
(1,425)	1:62:A:LEU:HD12	1:43:A:LEU:HA	4	0.21	0.05	0.2
(1,425)	1:62:A:LEU:HD13	1:43:A:LEU:HA	4	0.21	0.05	0.2
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE1	4	0.19	0.04	0.17
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE2	4	0.19	0.04	0.17
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE1	4	0.19	0.04	0.17
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE2	4	0.19	0.04	0.17
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE1	4	0.19	0.04	0.17
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE2	4	0.19	0.04	0.17
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD11	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD12	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD13	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD11	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD12	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD13	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD11	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD12	4	0.19	0.07	0.16
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD13	4	0.19	0.07	0.16
(1,40)	1:33:A:LEU:HD21	1:39:A:VAL:H	4	0.19	0.06	0.16
(1,40)	1:33:A:LEU:HD22	1:39:A:VAL:H	4	0.19	0.06	0.16
(1,40)	1:33:A:LEU:HD23	1:39:A:VAL:H	4	0.19	0.06	0.16
(1,506)	1:23:A:TRP:HD1	1:23:A:TRP:HA	4	0.18	0.04	0.18
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD21	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD22	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD23	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD21	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD22	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD23	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD21	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD22	4	0.18	0.04	0.2
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD23	4	0.18	0.04	0.2
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB1	4	0.18	0.08	0.14
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB2	4	0.18	0.08	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB3	4	0.18	0.08	0.14
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB1	4	0.18	0.08	0.14
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB2	4	0.18	0.08	0.14
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB3	4	0.18	0.08	0.14
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD2	4	0.16	0.05	0.14
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD3	4	0.16	0.05	0.14
(1,862)	1:74:A:ASN:HB2	1:138:A:ASN:HD21	4	0.16	0.02	0.16
(1,862)	1:74:A:ASN:HB3	1:138:A:ASN:HD21	4	0.16	0.02	0.16
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG21	4	0.16	0.04	0.15
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG22	4	0.16	0.04	0.15
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG23	4	0.16	0.04	0.15
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG21	4	0.15	0.03	0.15
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG22	4	0.15	0.03	0.15
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG23	4	0.15	0.03	0.15
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB2	4	0.15	0.05	0.14
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB3	4	0.15	0.05	0.14
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD1	4	0.15	0.05	0.12
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD2	4	0.15	0.05	0.12
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD1	4	0.15	0.05	0.12
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD2	4	0.15	0.05	0.12
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB1	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB2	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB3	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB1	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB2	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB3	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB1	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB2	4	0.14	0.02	0.14
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB3	4	0.14	0.02	0.14
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE2	4	0.14	0.06	0.11
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE3	4	0.14	0.06	0.11
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE2	4	0.14	0.06	0.11
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE3	4	0.14	0.06	0.11
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG21	4	0.14	0.04	0.12
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG22	4	0.14	0.04	0.12
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG23	4	0.14	0.04	0.12
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG21	4	0.14	0.04	0.12
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG22	4	0.14	0.04	0.12
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG23	4	0.14	0.04	0.12
(1,160)	1:156:A:ILE:HG21	1:153:A:ALA:HA	4	0.14	0.01	0.14
(1,160)	1:156:A:ILE:HG22	1:153:A:ALA:HA	4	0.14	0.01	0.14
(1,160)	1:156:A:ILE:HG23	1:153:A:ALA:HA	4	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,374)	1:62:A:LEU:HD21	1:69:A:ILE:H	4	0.14	0.05	0.11
(1,374)	1:62:A:LEU:HD22	1:69:A:ILE:H	4	0.14	0.05	0.11
(1,374)	1:62:A:LEU:HD23	1:69:A:ILE:H	4	0.14	0.05	0.11
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD1	4	0.13	0.02	0.12
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD2	4	0.13	0.02	0.12
(1,232)	1:92:A:ASN:HB2	1:93:A:LEU:HA	4	0.13	0.01	0.14
(1,232)	1:92:A:ASN:HB3	1:93:A:LEU:HA	4	0.13	0.01	0.14
(1,1248)	1:140:A:PHE:HA	1:102:A:SER:H	4	0.13	0.01	0.13
(1,334)	1:26:A:PRO:HB2	1:31:A:ALA:H	4	0.13	0.02	0.12
(1,334)	1:26:A:PRO:HB3	1:31:A:ALA:H	4	0.13	0.02	0.12
(1,1633)	1:156:A:ILE:HB	1:155:A:THR:H	4	0.13	0.01	0.12
(1,122)	1:114:A:GLN:HA	1:119:A:GLY:H	4	0.12	0.02	0.11
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB2	4	0.12	0.01	0.12
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB3	4	0.12	0.01	0.12
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB2	4	0.12	0.01	0.12
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB3	4	0.12	0.01	0.12
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB2	4	0.12	0.01	0.12
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB3	4	0.12	0.01	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD11	4	0.12	0.01	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD12	4	0.12	0.01	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD13	4	0.12	0.01	0.12
(1,2258)	1:137:A:ILE:HA	1:104:A:THR:H	4	0.12	0.02	0.12
(1,1310)	1:156:A:ILE:HB	1:157:A:GLU:H	4	0.12	0.0	0.12
(1,822)	1:70:A:LEU:HD21	1:113:A:VAL:HA	4	0.12	0.01	0.12
(1,822)	1:70:A:LEU:HD22	1:113:A:VAL:HA	4	0.12	0.01	0.12
(1,822)	1:70:A:LEU:HD23	1:113:A:VAL:HA	4	0.12	0.01	0.12
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD1	4	0.11	0.0	0.11
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD2	4	0.11	0.0	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD1	4	0.11	0.0	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD2	4	0.11	0.0	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD1	4	0.11	0.0	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD2	4	0.11	0.0	0.11
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD1	4	0.11	0.01	0.11
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD2	4	0.11	0.01	0.11
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD1	4	0.11	0.01	0.11
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD2	4	0.11	0.01	0.11
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD1	4	0.11	0.01	0.11
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD2	4	0.11	0.01	0.11
(1,704)	1:55:A:LEU:HG	1:55:A:LEU:HA	4	0.11	0.01	0.1
(1,1496)	1:161:A:GLY:H	1:159:A:LEU:H	3	0.32	0.01	0.33
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD11	3	0.26	0.08	0.31
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD12	3	0.26	0.08	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD13	3	0.26	0.08	0.31
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB1	3	0.25	0.02	0.24
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB2	3	0.25	0.02	0.24
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB3	3	0.25	0.02	0.24
(1,55)	1:45:A:VAL:HA	1:62:A:LEU:H	3	0.22	0.04	0.22
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD11	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD12	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD13	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD11	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD12	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD13	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD11	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD12	3	0.22	0.15	0.13
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD13	3	0.22	0.15	0.13
(1,1005)	1:98:A:ILE:HG21	1:143:A:PHE:H	3	0.22	0.13	0.15
(1,1005)	1:98:A:ILE:HG22	1:143:A:PHE:H	3	0.22	0.13	0.15
(1,1005)	1:98:A:ILE:HG23	1:143:A:PHE:H	3	0.22	0.13	0.15
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB2	3	0.22	0.04	0.21
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB3	3	0.22	0.04	0.21
(1,1736)	1:29:A:CYS:H	1:30:A:GLU:HA	3	0.21	0.01	0.21
(1,54)	1:23:A:TRP:H	1:24:A:LEU:H	3	0.2	0.06	0.18
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD1	3	0.19	0.04	0.21
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD2	3	0.19	0.04	0.21
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB2	3	0.18	0.1	0.12
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB3	3	0.18	0.1	0.12
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB2	3	0.18	0.1	0.12
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB3	3	0.18	0.1	0.12
(1,1758)	1:54:A:THR:HG21	1:55:A:LEU:H	3	0.18	0.07	0.16
(1,1758)	1:54:A:THR:HG22	1:55:A:LEU:H	3	0.18	0.07	0.16
(1,1758)	1:54:A:THR:HG23	1:55:A:LEU:H	3	0.18	0.07	0.16
(1,676)	1:48:A:ILE:HB	1:48:A:ILE:H	3	0.17	0.04	0.2
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD2	3	0.17	0.05	0.18
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD3	3	0.17	0.05	0.18
(1,1801)	1:41:A:LYS:HD2	1:42:A:VAL:H	3	0.17	0.06	0.14
(1,1801)	1:41:A:LYS:HD3	1:42:A:VAL:H	3	0.17	0.06	0.14
(1,462)	1:8:A:SER:HB2	1:10:A:ASP:H	3	0.16	0.04	0.14
(1,462)	1:8:A:SER:HB3	1:10:A:ASP:H	3	0.16	0.04	0.14
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG21	3	0.16	0.05	0.17
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG22	3	0.16	0.05	0.17
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG23	3	0.16	0.05	0.17
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG21	3	0.16	0.05	0.17
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG22	3	0.16	0.05	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG23	3	0.16	0.05	0.17
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG21	3	0.16	0.05	0.17
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG22	3	0.16	0.05	0.17
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG23	3	0.16	0.05	0.17
(1,1016)	1:99:A:MET:HE1	1:143:A:PHE:HZ	3	0.16	0.04	0.15
(1,1016)	1:99:A:MET:HE2	1:143:A:PHE:HZ	3	0.16	0.04	0.15
(1,1016)	1:99:A:MET:HE3	1:143:A:PHE:HZ	3	0.16	0.04	0.15
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG2	3	0.16	0.07	0.11
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG3	3	0.16	0.07	0.11
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD1	3	0.16	0.04	0.14
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD2	3	0.16	0.04	0.14
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD1	3	0.16	0.04	0.14
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD2	3	0.16	0.04	0.14
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD1	3	0.16	0.04	0.14
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD2	3	0.16	0.04	0.14
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG2	3	0.15	0.04	0.15
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG3	3	0.15	0.04	0.15
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD2	3	0.15	0.03	0.15
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD3	3	0.15	0.03	0.15
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD2	3	0.15	0.03	0.15
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD3	3	0.15	0.03	0.15
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD2	3	0.15	0.03	0.15
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD3	3	0.15	0.03	0.15
(1,637)	1:42:A:VAL:HG21	1:99:A:MET:HA	3	0.14	0.02	0.14
(1,637)	1:42:A:VAL:HG22	1:99:A:MET:HA	3	0.14	0.02	0.14
(1,637)	1:42:A:VAL:HG23	1:99:A:MET:HA	3	0.14	0.02	0.14
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD11	3	0.14	0.02	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD12	3	0.14	0.02	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD13	3	0.14	0.02	0.12
(1,1918)	1:13:A:ARG:H	1:12:A:VAL:HB	3	0.14	0.02	0.12
(1,655)	1:42:A:VAL:HG21	1:100:A:ILE:H	3	0.13	0.02	0.14
(1,655)	1:42:A:VAL:HG22	1:100:A:ILE:H	3	0.13	0.02	0.14
(1,655)	1:42:A:VAL:HG23	1:100:A:ILE:H	3	0.13	0.02	0.14
(1,701)	1:55:A:LEU:HD21	1:55:A:LEU:H	3	0.13	0.0	0.13
(1,701)	1:55:A:LEU:HD22	1:55:A:LEU:H	3	0.13	0.0	0.13
(1,701)	1:55:A:LEU:HD23	1:55:A:LEU:H	3	0.13	0.0	0.13
(1,854)	1:73:A:ALA:HB1	1:140:A:PHE:HZ	3	0.13	0.02	0.12
(1,854)	1:73:A:ALA:HB2	1:140:A:PHE:HZ	3	0.13	0.02	0.12
(1,854)	1:73:A:ALA:HB3	1:140:A:PHE:HZ	3	0.13	0.02	0.12
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD1	3	0.13	0.02	0.12
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD2	3	0.13	0.02	0.12
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD1	3	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD2	3	0.13	0.02	0.12
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD1	3	0.13	0.02	0.12
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD2	3	0.13	0.02	0.12
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD11	3	0.13	0.02	0.14
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD12	3	0.13	0.02	0.14
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD13	3	0.13	0.02	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD21	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD22	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD23	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD21	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD22	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD23	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD21	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD22	3	0.13	0.01	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD23	3	0.13	0.01	0.14
(1,364)	1:47:A:ARG:HD2	1:61:A:CYS:H	3	0.13	0.03	0.11
(1,364)	1:47:A:ARG:HD3	1:61:A:CYS:H	3	0.13	0.03	0.11
(1,974)	1:45:A:VAL:HG21	1:95:A:ASN:H	3	0.13	0.02	0.12
(1,974)	1:45:A:VAL:HG22	1:95:A:ASN:H	3	0.13	0.02	0.12
(1,974)	1:45:A:VAL:HG23	1:95:A:ASN:H	3	0.13	0.02	0.12
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD1	3	0.13	0.01	0.13
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD2	3	0.13	0.01	0.13
(1,2180)	1:140:A:PHE:HD1	1:142:A:MET:H	3	0.13	0.02	0.12
(1,2180)	1:140:A:PHE:HD2	1:142:A:MET:H	3	0.13	0.02	0.12
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD1	3	0.12	0.02	0.13
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD2	3	0.12	0.02	0.13
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD1	3	0.12	0.02	0.13
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD2	3	0.12	0.02	0.13
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD11	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD12	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD13	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD11	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD12	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD13	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD11	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD12	3	0.12	0.0	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD13	3	0.12	0.0	0.12
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD1	3	0.12	0.02	0.11
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD2	3	0.12	0.02	0.11
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG21	3	0.12	0.0	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG22	3	0.12	0.0	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG23	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG21	3	0.12	0.0	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG22	3	0.12	0.0	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG23	3	0.12	0.0	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG21	3	0.12	0.0	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG22	3	0.12	0.0	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG23	3	0.12	0.0	0.12
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG21	3	0.12	0.01	0.12
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG22	3	0.12	0.01	0.12
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG23	3	0.12	0.01	0.12
(1,306)	1:108:A:TYR:HE1	1:112:A:GLN:HA	3	0.11	0.0	0.11
(1,306)	1:108:A:TYR:HE2	1:112:A:GLN:HA	3	0.11	0.0	0.11
(1,412)	1:137:A:ILE:HD11	1:71:A:ALA:H	3	0.11	0.0	0.11
(1,412)	1:137:A:ILE:HD12	1:71:A:ALA:H	3	0.11	0.0	0.11
(1,412)	1:137:A:ILE:HD13	1:71:A:ALA:H	3	0.11	0.0	0.11
(1,50)	1:150:A:LEU:HD21	1:64:A:ASP:HA	3	0.11	0.01	0.11
(1,50)	1:150:A:LEU:HD22	1:64:A:ASP:HA	3	0.11	0.01	0.11
(1,50)	1:150:A:LEU:HD23	1:64:A:ASP:HA	3	0.11	0.01	0.11
(1,354)	1:158:A:PHE:HA	1:160:A:TYR:H	2	0.34	0.04	0.34
(1,1851)	1:146:A:ASP:H	1:145:A:ARG:H	2	0.34	0.05	0.34
(1,1497)	1:161:A:GLY:H	1:160:A:TYR:HD1	2	0.28	0.07	0.28
(1,1497)	1:161:A:GLY:H	1:160:A:TYR:HD2	2	0.28	0.07	0.28
(1,1820)	1:175:A:SER:H	1:174:A:PHE:H	2	0.24	0.11	0.24
(1,1640)	1:86:A:ARG:H	1:86:A:ARG:HG2	2	0.22	0.11	0.22
(1,1640)	1:86:A:ARG:H	1:86:A:ARG:HG3	2	0.22	0.11	0.22
(1,1853)	1:173:A:GLU:H	1:172:A:GLN:HB2	2	0.22	0.04	0.22
(1,1853)	1:173:A:GLU:H	1:172:A:GLN:HB3	2	0.22	0.04	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD11	2	0.22	0.0	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD12	2	0.22	0.0	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD13	2	0.22	0.0	0.22
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD11	2	0.22	0.01	0.22
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD12	2	0.22	0.01	0.22
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD13	2	0.22	0.01	0.22
(1,1621)	1:91:A:GLN:HE21	1:88:A:ARG:HA	2	0.21	0.06	0.21
(1,1779)	1:20:A:MET:H	1:20:A:MET:HG2	2	0.21	0.02	0.21
(1,1779)	1:20:A:MET:H	1:20:A:MET:HG3	2	0.21	0.02	0.21
(1,520)	1:24:A:LEU:HD21	1:23:A:TRP:HZ2	2	0.21	0.08	0.21
(1,520)	1:24:A:LEU:HD22	1:23:A:TRP:HZ2	2	0.21	0.08	0.21
(1,520)	1:24:A:LEU:HD23	1:23:A:TRP:HZ2	2	0.21	0.08	0.21
(1,161)	1:156:A:ILE:HG21	1:63:A:CYS:HB2	2	0.2	0.02	0.2
(1,161)	1:156:A:ILE:HG21	1:63:A:CYS:HB3	2	0.2	0.02	0.2
(1,161)	1:156:A:ILE:HG22	1:63:A:CYS:HB2	2	0.2	0.02	0.2
(1,161)	1:156:A:ILE:HG22	1:63:A:CYS:HB3	2	0.2	0.02	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,161)	1:156:A:ILE:HG23	1:63:A:CYS:HB2	2	0.2	0.02	0.2
(1,161)	1:156:A:ILE:HG23	1:63:A:CYS:HB3	2	0.2	0.02	0.2
(1,1107)	1:113:A:VAL:HG21	1:114:A:GLN:HE22	2	0.2	0.06	0.2
(1,1107)	1:113:A:VAL:HG22	1:114:A:GLN:HE22	2	0.2	0.06	0.2
(1,1107)	1:113:A:VAL:HG23	1:114:A:GLN:HE22	2	0.2	0.06	0.2
(1,8)	1:96:A:SER:HA	1:147:A:GLN:HG2	2	0.19	0.06	0.19
(1,8)	1:96:A:SER:HA	1:147:A:GLN:HG3	2	0.19	0.06	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD21	2	0.19	0.0	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD22	2	0.19	0.0	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD23	2	0.19	0.0	0.19
(1,28)	1:105:A:ILE:HG12	1:169:A:PHE:HE1	2	0.18	0.02	0.18
(1,28)	1:105:A:ILE:HG12	1:169:A:PHE:HE2	2	0.18	0.02	0.18
(1,28)	1:105:A:ILE:HG13	1:169:A:PHE:HE1	2	0.18	0.02	0.18
(1,28)	1:105:A:ILE:HG13	1:169:A:PHE:HE2	2	0.18	0.02	0.18
(1,1547)	1:168:A:ARG:H	1:169:A:PHE:HD1	2	0.18	0.02	0.18
(1,1547)	1:168:A:ARG:H	1:169:A:PHE:HD2	2	0.18	0.02	0.18
(1,288)	1:31:A:ALA:HB1	1:33:A:LEU:HB2	2	0.18	0.06	0.18
(1,288)	1:31:A:ALA:HB1	1:33:A:LEU:HB3	2	0.18	0.06	0.18
(1,288)	1:31:A:ALA:HB2	1:33:A:LEU:HB2	2	0.18	0.06	0.18
(1,288)	1:31:A:ALA:HB2	1:33:A:LEU:HB3	2	0.18	0.06	0.18
(1,288)	1:31:A:ALA:HB3	1:33:A:LEU:HB2	2	0.18	0.06	0.18
(1,288)	1:31:A:ALA:HB3	1:33:A:LEU:HB3	2	0.18	0.06	0.18
(1,614)	1:41:A:LYS:HA	1:41:A:LYS:HD2	2	0.18	0.04	0.18
(1,614)	1:41:A:LYS:HA	1:41:A:LYS:HD3	2	0.18	0.04	0.18
(1,615)	1:41:A:LYS:HD2	1:41:A:LYS:HA	2	0.18	0.04	0.18
(1,615)	1:41:A:LYS:HD3	1:41:A:LYS:HA	2	0.18	0.04	0.18
(1,703)	1:55:A:LEU:HG	1:55:A:LEU:H	2	0.18	0.04	0.18
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD11	2	0.18	0.03	0.18
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD12	2	0.18	0.03	0.18
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD13	2	0.18	0.03	0.18
(1,284)	1:39:A:VAL:HG21	1:40:A:ASP:HA	2	0.17	0.06	0.17
(1,284)	1:39:A:VAL:HG22	1:40:A:ASP:HA	2	0.17	0.06	0.17
(1,284)	1:39:A:VAL:HG23	1:40:A:ASP:HA	2	0.17	0.06	0.17
(1,2179)	1:142:A:MET:H	1:84:A:LYS:HB2	2	0.17	0.02	0.17
(1,2179)	1:142:A:MET:H	1:84:A:LYS:HB3	2	0.17	0.02	0.17
(1,1350)	1:159:A:LEU:HD21	1:160:A:TYR:HB2	2	0.16	0.06	0.16
(1,1350)	1:159:A:LEU:HD21	1:160:A:TYR:HB3	2	0.16	0.06	0.16
(1,1350)	1:159:A:LEU:HD22	1:160:A:TYR:HB2	2	0.16	0.06	0.16
(1,1350)	1:159:A:LEU:HD22	1:160:A:TYR:HB3	2	0.16	0.06	0.16
(1,1350)	1:159:A:LEU:HD23	1:160:A:TYR:HB2	2	0.16	0.06	0.16
(1,1350)	1:159:A:LEU:HD23	1:160:A:TYR:HB3	2	0.16	0.06	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD11	2	0.16	0.0	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD12	2	0.16	0.0	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD13	2	0.16	0.0	0.16
(1,1482)	1:121:A:LYS:HE2	1:114:A:GLN:HE22	2	0.16	0.04	0.16
(1,1482)	1:121:A:LYS:HE3	1:114:A:GLN:HE22	2	0.16	0.04	0.16
(1,1808)	1:129:A:PHE:H	1:128:A:LEU:HB2	2	0.16	0.05	0.16
(1,1808)	1:129:A:PHE:H	1:128:A:LEU:HB3	2	0.16	0.05	0.16
(1,281)	1:42:A:VAL:HB	1:20:A:MET:HG2	2	0.15	0.02	0.15
(1,281)	1:42:A:VAL:HB	1:20:A:MET:HG3	2	0.15	0.02	0.15
(1,148)	1:167:A:ALA:HB1	1:164:A:ARG:HD2	2	0.15	0.0	0.15
(1,148)	1:167:A:ALA:HB1	1:164:A:ARG:HD3	2	0.15	0.0	0.15
(1,148)	1:167:A:ALA:HB2	1:164:A:ARG:HD2	2	0.15	0.0	0.15
(1,148)	1:167:A:ALA:HB2	1:164:A:ARG:HD3	2	0.15	0.0	0.15
(1,148)	1:167:A:ALA:HB3	1:164:A:ARG:HD2	2	0.15	0.0	0.15
(1,148)	1:167:A:ALA:HB3	1:164:A:ARG:HD3	2	0.15	0.0	0.15
(1,341)	1:20:A:MET:HE1	1:66:A:ASN:H	2	0.15	0.03	0.15
(1,341)	1:20:A:MET:HE2	1:66:A:ASN:H	2	0.15	0.03	0.15
(1,341)	1:20:A:MET:HE3	1:66:A:ASN:H	2	0.15	0.03	0.15
(1,499)	1:20:A:MET:HE1	1:65:A:ALA:HA	2	0.15	0.04	0.15
(1,499)	1:20:A:MET:HE2	1:65:A:ALA:HA	2	0.15	0.04	0.15
(1,499)	1:20:A:MET:HE3	1:65:A:ALA:HA	2	0.15	0.04	0.15
(1,601)	1:39:A:VAL:HG11	1:39:A:VAL:H	2	0.15	0.03	0.15
(1,601)	1:39:A:VAL:HG12	1:39:A:VAL:H	2	0.15	0.03	0.15
(1,601)	1:39:A:VAL:HG13	1:39:A:VAL:H	2	0.15	0.03	0.15
(1,359)	1:42:A:VAL:HB	1:20:A:MET:HA	2	0.14	0.03	0.14
(1,150)	1:166:A:ILE:HG21	1:170:A:ILE:H	2	0.14	0.01	0.14
(1,150)	1:166:A:ILE:HG22	1:170:A:ILE:H	2	0.14	0.01	0.14
(1,150)	1:166:A:ILE:HG23	1:170:A:ILE:H	2	0.14	0.01	0.14
(1,251)	1:76:A:LYS:HG2	1:74:A:ASN:HD21	2	0.14	0.01	0.14
(1,251)	1:76:A:LYS:HG2	1:74:A:ASN:HD22	2	0.14	0.01	0.14
(1,251)	1:76:A:LYS:HG3	1:74:A:ASN:HD21	2	0.14	0.01	0.14
(1,251)	1:76:A:LYS:HG3	1:74:A:ASN:HD22	2	0.14	0.01	0.14
(1,631)	1:42:A:VAL:HG11	1:143:A:PHE:HD1	2	0.14	0.01	0.14
(1,631)	1:42:A:VAL:HG11	1:143:A:PHE:HD2	2	0.14	0.01	0.14
(1,631)	1:42:A:VAL:HG12	1:143:A:PHE:HD1	2	0.14	0.01	0.14
(1,631)	1:42:A:VAL:HG12	1:143:A:PHE:HD2	2	0.14	0.01	0.14
(1,631)	1:42:A:VAL:HG13	1:143:A:PHE:HD1	2	0.14	0.01	0.14
(1,631)	1:42:A:VAL:HG13	1:143:A:PHE:HD2	2	0.14	0.01	0.14
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD21	2	0.14	0.02	0.14
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD22	2	0.14	0.02	0.14
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD23	2	0.14	0.02	0.14
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD21	2	0.14	0.02	0.14
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD22	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD23	2	0.14	0.02	0.14
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD21	2	0.14	0.02	0.14
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD22	2	0.14	0.02	0.14
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD23	2	0.14	0.02	0.14
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB1	2	0.14	0.02	0.14
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB2	2	0.14	0.02	0.14
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB3	2	0.14	0.02	0.14
(1,1726)	1:166:A:ILE:HA	1:171:A:GLU:H	2	0.14	0.02	0.14
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD21	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD22	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD23	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD21	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD22	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD23	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD21	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD22	2	0.13	0.02	0.13
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD23	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG21	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG22	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG23	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG21	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG22	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG23	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG21	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG22	2	0.13	0.02	0.13
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG23	2	0.13	0.02	0.13
(1,164)	1:156:A:ILE:HD11	1:66:A:ASN:HA	2	0.12	0.02	0.12
(1,164)	1:156:A:ILE:HD12	1:66:A:ASN:HA	2	0.12	0.02	0.12
(1,164)	1:156:A:ILE:HD13	1:66:A:ASN:HA	2	0.12	0.02	0.12
(1,680)	1:48:A:ILE:HD11	1:90:A:THR:HA	2	0.12	0.01	0.12
(1,680)	1:48:A:ILE:HD12	1:90:A:THR:HA	2	0.12	0.01	0.12
(1,680)	1:48:A:ILE:HD13	1:90:A:THR:HA	2	0.12	0.01	0.12
(1,756)	1:64:A:ASP:HA	1:23:A:TRP:HE1	2	0.12	0.01	0.12
(1,1999)	1:149:A:ILE:HD11	1:149:A:ILE:H	2	0.12	0.02	0.12
(1,1999)	1:149:A:ILE:HD12	1:149:A:ILE:H	2	0.12	0.02	0.12
(1,1999)	1:149:A:ILE:HD13	1:149:A:ILE:H	2	0.12	0.02	0.12
(1,2141)	1:65:A:ALA:HB1	1:67:A:TYR:H	2	0.12	0.01	0.12
(1,2141)	1:65:A:ALA:HB2	1:67:A:TYR:H	2	0.12	0.01	0.12
(1,2141)	1:65:A:ALA:HB3	1:67:A:TYR:H	2	0.12	0.01	0.12
(1,155)	1:162:A:THR:HG21	1:67:A:TYR:HB2	2	0.12	0.01	0.12
(1,155)	1:162:A:THR:HG21	1:67:A:TYR:HB3	2	0.12	0.01	0.12
(1,155)	1:162:A:THR:HG22	1:67:A:TYR:HB2	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,155)	1:162:A:THR:HG22	1:67:A:TYR:HB3	2	0.12	0.01	0.12
(1,155)	1:162:A:THR:HG23	1:67:A:TYR:HB2	2	0.12	0.01	0.12
(1,155)	1:162:A:THR:HG23	1:67:A:TYR:HB3	2	0.12	0.01	0.12
(1,1481)	1:124:A:GLN:HE22	1:129:A:PHE:HE1	2	0.12	0.0	0.12
(1,1481)	1:124:A:GLN:HE22	1:129:A:PHE:HE2	2	0.12	0.0	0.12
(1,2004)	1:78:A:ILE:H	1:140:A:PHE:HE1	2	0.12	0.01	0.12
(1,2004)	1:78:A:ILE:H	1:140:A:PHE:HE2	2	0.12	0.01	0.12
(1,388)	1:85:A:GLU:HA	1:87:A:ARG:H	2	0.12	0.02	0.12
(1,1348)	1:159:A:LEU:HD21	1:159:A:LEU:H	2	0.12	0.02	0.12
(1,1348)	1:159:A:LEU:HD22	1:159:A:LEU:H	2	0.12	0.02	0.12
(1,1348)	1:159:A:LEU:HD23	1:159:A:LEU:H	2	0.12	0.02	0.12
(1,922)	1:83:A:ARG:HA	1:83:A:ARG:HD2	2	0.12	0.0	0.12
(1,922)	1:83:A:ARG:HA	1:83:A:ARG:HD3	2	0.12	0.0	0.12
(1,89)	1:135:A:LEU:HD11	1:23:A:TRP:HZ3	2	0.11	0.0	0.11
(1,89)	1:135:A:LEU:HD12	1:23:A:TRP:HZ3	2	0.11	0.0	0.11
(1,89)	1:135:A:LEU:HD13	1:23:A:TRP:HZ3	2	0.11	0.0	0.11
(1,130)	1:134:A:VAL:HG11	1:116:A:PHE:HE1	2	0.11	0.0	0.11
(1,130)	1:134:A:VAL:HG11	1:116:A:PHE:HE2	2	0.11	0.0	0.11
(1,130)	1:134:A:VAL:HG12	1:116:A:PHE:HE1	2	0.11	0.0	0.11
(1,130)	1:134:A:VAL:HG12	1:116:A:PHE:HE2	2	0.11	0.0	0.11
(1,130)	1:134:A:VAL:HG13	1:116:A:PHE:HE1	2	0.11	0.0	0.11
(1,130)	1:134:A:VAL:HG13	1:116:A:PHE:HE2	2	0.11	0.0	0.11
(1,295)	1:27:A:VAL:HG21	1:23:A:TRP:HE3	2	0.11	0.0	0.11
(1,295)	1:27:A:VAL:HG22	1:23:A:TRP:HE3	2	0.11	0.0	0.11
(1,295)	1:27:A:VAL:HG23	1:23:A:TRP:HE3	2	0.11	0.0	0.11
(1,366)	1:162:A:THR:HG21	1:157:A:GLU:HB2	2	0.11	0.0	0.11
(1,366)	1:162:A:THR:HG21	1:157:A:GLU:HB3	2	0.11	0.0	0.11
(1,366)	1:162:A:THR:HG22	1:157:A:GLU:HB2	2	0.11	0.0	0.11
(1,366)	1:162:A:THR:HG22	1:157:A:GLU:HB3	2	0.11	0.0	0.11
(1,366)	1:162:A:THR:HG23	1:157:A:GLU:HB2	2	0.11	0.0	0.11
(1,366)	1:162:A:THR:HG23	1:157:A:GLU:HB3	2	0.11	0.0	0.11
(1,1357)	1:162:A:THR:HG21	1:161:A:GLY:H	2	0.11	0.0	0.11
(1,1357)	1:162:A:THR:HG22	1:161:A:GLY:H	2	0.11	0.0	0.11
(1,1357)	1:162:A:THR:HG23	1:161:A:GLY:H	2	0.11	0.0	0.11

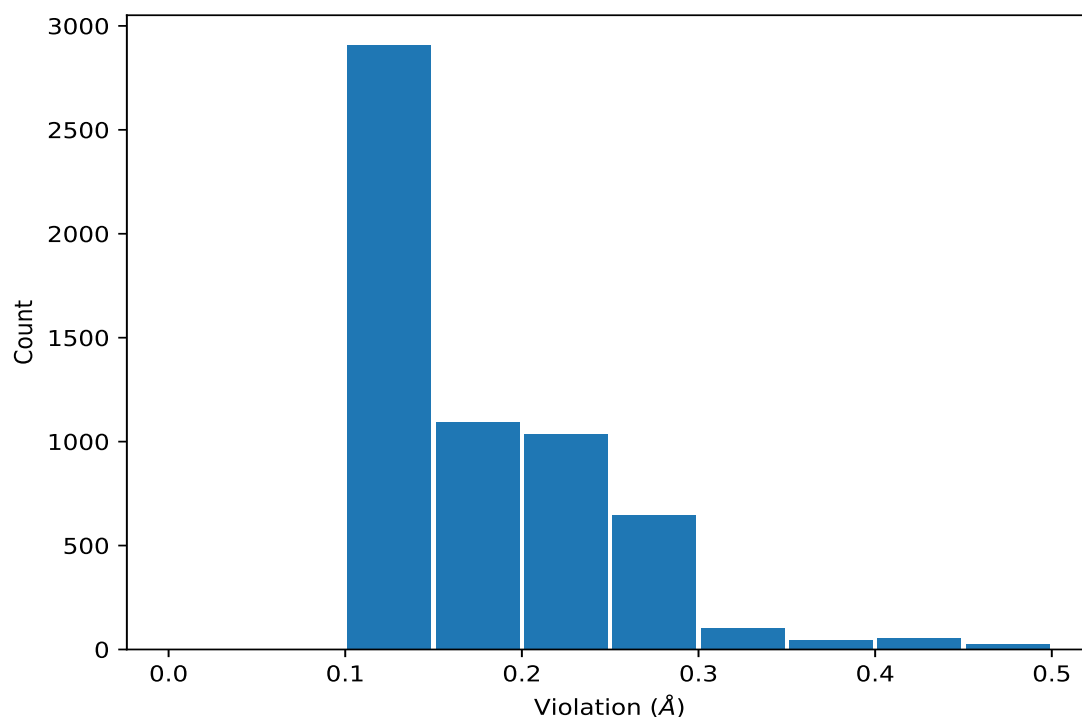
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation



## 9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:34:A:GLY:HA2	1:36:A:ASN:H	18	0.5
(1,578)	1:34:A:GLY:HA3	1:36:A:ASN:H	18	0.5
(1,1850)	1:172:A:GLN:H	1:173:A:GLU:H	20	0.49
(1,1564)	1:74:A:ASN:H	1:137:A:ILE:HG12	16	0.49
(1,1564)	1:74:A:ASN:H	1:137:A:ILE:HG13	16	0.49
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	1	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	1	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	2	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	2	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	6	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	8	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	8	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	12	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	12	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	15	0.48
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	15	0.48
(1,1727)	1:171:A:GLU:H	1:171:A:GLU:HG2	2	0.47
(1,1727)	1:171:A:GLU:H	1:171:A:GLU:HG3	2	0.47
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG2	4	0.47
(1,526)	1:26:A:PRO:HA	1:26:A:PRO:HG3	4	0.47
(1,327)	1:127:A:SER:HB2	1:129:A:PHE:H	11	0.47
(1,327)	1:127:A:SER:HB3	1:129:A:PHE:H	11	0.47
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	14	0.47
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	14	0.47
(1,492)	1:19:A:HIS:HA	1:19:A:HIS:HD2	7	0.44
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	14	0.44
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	14	0.44
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	14	0.44
(1,410)	1:171:A:GLU:HG2	1:168:A:ARG:H	2	0.44
(1,410)	1:171:A:GLU:HG3	1:168:A:ARG:H	2	0.44
(1,350)	1:144:A:ASN:HB2	1:97:A:GLU:HB2	20	0.44
(1,350)	1:144:A:ASN:HB2	1:97:A:GLU:HB3	20	0.44
(1,350)	1:144:A:ASN:HB3	1:97:A:GLU:HB2	20	0.44
(1,350)	1:144:A:ASN:HB3	1:97:A:GLU:HB3	20	0.44
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	5	0.43
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD11	2	0.43
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD12	2	0.43
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD13	2	0.43
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD11	2	0.43
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD12	2	0.43
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD13	2	0.43
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD11	2	0.43
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD12	2	0.43
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD13	2	0.43
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD1	7	0.43
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD2	7	0.43
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD1	7	0.43
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD2	7	0.43
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD1	7	0.43
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD2	7	0.43
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD1	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD2	17	0.43
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD1	17	0.43
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD2	17	0.43
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD1	17	0.43
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD2	17	0.43
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	10	0.41
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	10	0.41
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	10	0.41
(1,1005)	1:98:A:ILE:HG21	1:143:A:PHE:H	20	0.41
(1,1005)	1:98:A:ILE:HG22	1:143:A:PHE:H	20	0.41
(1,1005)	1:98:A:ILE:HG23	1:143:A:PHE:H	20	0.41
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	14	0.41
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	14	0.41
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	14	0.41
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	9	0.4
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	9	0.4
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	9	0.4
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	17	0.4
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	17	0.4
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	17	0.4
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	17	0.4
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	17	0.4
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	17	0.4
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB2	14	0.4
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB3	14	0.4
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB2	14	0.4
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB3	14	0.4
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB2	14	0.4
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB3	14	0.4
(1,2073)	1:128:A:LEU:HD11	1:128:A:LEU:H	11	0.39
(1,2073)	1:128:A:LEU:HD12	1:128:A:LEU:H	11	0.39
(1,2073)	1:128:A:LEU:HD13	1:128:A:LEU:H	11	0.39
(1,1851)	1:146:A:ASP:H	1:145:A:ARG:H	14	0.39
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	19	0.39
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	19	0.39
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	19	0.39
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	13	0.39
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	13	0.39
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	13	0.39
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD1	19	0.39
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD2	19	0.39
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD1	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD2	13	0.39
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD1	13	0.39
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD2	13	0.39
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD1	13	0.39
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD2	13	0.39
(1,958)	1:90:A:THR:HB	1:91:A:GLN:H	14	0.38
(1,454)	1:159:A:LEU:HA	1:67:A:TYR:HA	1	0.38
(1,354)	1:158:A:PHE:HA	1:160:A:TYR:H	15	0.38
(1,2155)	1:136:A:GLU:H	1:137:A:ILE:HD11	16	0.37
(1,2155)	1:136:A:GLU:H	1:137:A:ILE:HD12	16	0.37
(1,2155)	1:136:A:GLU:H	1:137:A:ILE:HD13	16	0.37
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	20	0.37
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	20	0.37
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	20	0.37
(1,1491)	1:36:A:ASN:HA	1:36:A:ASN:HD22	9	0.37
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	2	0.37
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	2	0.37
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	2	0.37
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	14	0.37
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	14	0.37
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	14	0.37
(1,1868)	1:15:A:THR:HG21	1:15:A:THR:H	13	0.36
(1,1868)	1:15:A:THR:HG22	1:15:A:THR:H	13	0.36
(1,1868)	1:15:A:THR:HG23	1:15:A:THR:H	13	0.36
(1,1514)	1:120:A:LEU:H	1:114:A:GLN:HG2	5	0.36
(1,1514)	1:120:A:LEU:H	1:114:A:GLN:HG3	5	0.36
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	3	0.36
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	3	0.36
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	3	0.36
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	16	0.36
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	16	0.36
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	16	0.36
(1,1820)	1:175:A:SER:H	1:174:A:PHE:H	19	0.35
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	11	0.35
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	11	0.35
(1,1497)	1:161:A:GLY:H	1:160:A:TYR:HD1	5	0.35
(1,1497)	1:161:A:GLY:H	1:160:A:TYR:HD2	5	0.35
(1,958)	1:90:A:THR:HB	1:91:A:GLN:H	3	0.35
(1,958)	1:90:A:THR:HB	1:91:A:GLN:H	19	0.35
(1,678)	1:48:A:ILE:HD11	1:48:A:ILE:H	17	0.35
(1,678)	1:48:A:ILE:HD12	1:48:A:ILE:H	17	0.35
(1,678)	1:48:A:ILE:HD13	1:48:A:ILE:H	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:86:A:ARG:HG2	1:86:A:ARG:HA	13	0.35
(1,389)	1:86:A:ARG:HG3	1:86:A:ARG:HA	13	0.35
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	2	0.35
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	2	0.35
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	19	0.35
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	19	0.35
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	19	0.35
(1,958)	1:90:A:THR:HB	1:91:A:GLN:H	16	0.34
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	9	0.34
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	9	0.34
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	9	0.34
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	9	0.34
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	9	0.34
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	9	0.34
(1,1879)	1:177:A:GLU:H	1:175:A:SER:HB2	9	0.33
(1,1879)	1:177:A:GLU:H	1:175:A:SER:HB3	9	0.33
(1,1640)	1:86:A:ARG:H	1:86:A:ARG:HG2	13	0.33
(1,1640)	1:86:A:ARG:H	1:86:A:ARG:HG3	13	0.33
(1,1496)	1:161:A:GLY:H	1:159:A:LEU:H	5	0.33
(1,1496)	1:161:A:GLY:H	1:159:A:LEU:H	9	0.33
(1,700)	1:55:A:LEU:HD11	1:55:A:LEU:H	16	0.33
(1,700)	1:55:A:LEU:HD12	1:55:A:LEU:H	16	0.33
(1,700)	1:55:A:LEU:HD13	1:55:A:LEU:H	16	0.33
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	16	0.33
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	16	0.33
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	16	0.33
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	14	0.33
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	14	0.33
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	14	0.33
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD11	7	0.32
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD12	7	0.32
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD13	7	0.32
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	1	0.32
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	1	0.32
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	1	0.32
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD21	4	0.32
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD22	4	0.32
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD23	4	0.32
(1,1447)	1:177:A:GLU:HA	1:177:A:GLU:HG2	15	0.32
(1,1447)	1:177:A:GLU:HA	1:177:A:GLU:HG3	15	0.32
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	2	0.32
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	2	0.32
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	2	0.32
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	2	0.32
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	2	0.32
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	20	0.32
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	20	0.32
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	20	0.32
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	11	0.32
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	11	0.32
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB1	1	0.32
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB2	1	0.32
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB3	1	0.32
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB1	1	0.32
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB2	1	0.32
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB3	1	0.32
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	5	0.32
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB2	2	0.32
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB3	2	0.32
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB2	2	0.32
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB3	2	0.32
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	5	0.32
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	5	0.32
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	5	0.32
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD11	17	0.31
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD12	17	0.31
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD13	17	0.31
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	7	0.31
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	7	0.31
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	2	0.31
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	2	0.31
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	2	0.31
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD21	20	0.31
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD22	20	0.31
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD23	20	0.31
(1,1496)	1:161:A:GLY:H	1:159:A:LEU:H	15	0.31
(1,1325)	1:157:A:GLU:HA	1:157:A:GLU:HG2	3	0.31
(1,1325)	1:157:A:GLU:HA	1:157:A:GLU:HG3	3	0.31
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	16	0.31
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	16	0.31
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	16	0.31
(1,963)	1:92:A:ASN:HA	1:92:A:ASN:HD22	2	0.31
(1,409)	1:171:A:GLU:HB2	1:172:A:GLN:H	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:171:A:GLU:HB3	1:172:A:GLN:H	20	0.31
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD11	16	0.31
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD12	16	0.31
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD13	16	0.31
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD11	16	0.31
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD12	16	0.31
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD13	16	0.31
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD11	16	0.31
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD12	16	0.31
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD13	16	0.31
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	20	0.3
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	20	0.3
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	20	0.3
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	18	0.3
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	6	0.3
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	6	0.3
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	6	0.3
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	12	0.3
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	12	0.3
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	12	0.3
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD21	15	0.3
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD22	15	0.3
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD23	15	0.3
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	15	0.3
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	15	0.3
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	15	0.3
(1,1233)	1:137:A:ILE:HD11	1:137:A:ILE:HG21	16	0.3
(1,1233)	1:137:A:ILE:HD11	1:137:A:ILE:HG22	16	0.3
(1,1233)	1:137:A:ILE:HD11	1:137:A:ILE:HG23	16	0.3
(1,1233)	1:137:A:ILE:HD12	1:137:A:ILE:HG21	16	0.3
(1,1233)	1:137:A:ILE:HD12	1:137:A:ILE:HG22	16	0.3
(1,1233)	1:137:A:ILE:HD12	1:137:A:ILE:HG23	16	0.3
(1,1233)	1:137:A:ILE:HD13	1:137:A:ILE:HG21	16	0.3
(1,1233)	1:137:A:ILE:HD13	1:137:A:ILE:HG22	16	0.3
(1,1233)	1:137:A:ILE:HD13	1:137:A:ILE:HG23	16	0.3
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	2	0.3
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	2	0.3
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	2	0.3
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	19	0.3
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	19	0.3
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	19	0.3
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	8	0.3
(1,354)	1:158:A:PHE:HA	1:160:A:TYR:H	9	0.3
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	15	0.3
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	15	0.3
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	15	0.3
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	2	0.29
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	2	0.29
(1,1851)	1:146:A:ASP:H	1:145:A:ARG:H	20	0.29
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	19	0.29
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	19	0.29
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	19	0.29
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD21	5	0.29
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD22	5	0.29
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD23	5	0.29
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	6	0.29
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	6	0.29
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	6	0.29
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	8	0.29
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	8	0.29
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	8	0.29
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	12	0.29
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	12	0.29
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	12	0.29
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	13	0.29
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	13	0.29
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	13	0.29
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	19	0.29
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	19	0.29
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	19	0.29
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	11	0.29
(1,1091)	1:111:A:ASP:HB2	1:112:A:GLN:H	9	0.29
(1,1091)	1:111:A:ASP:HB3	1:112:A:GLN:H	9	0.29
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	1	0.29
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	1	0.29
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	1	0.29
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	16	0.29
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	16	0.29
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	16	0.29
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	20	0.29
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	20	0.29
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	20	0.29
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	20	0.29
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	20	0.29
(1,963)	1:92:A:ASN:HA	1:92:A:ASN:HD22	7	0.29
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	5	0.29
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	5	0.29
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	5	0.29
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	8	0.29
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	8	0.29
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	8	0.29
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	9	0.29
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	9	0.29
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	9	0.29
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	10	0.29
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	10	0.29
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	10	0.29
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	11	0.29
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	11	0.29
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	11	0.29
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	13	0.29
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	13	0.29
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	13	0.29
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	15	0.29
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	15	0.29
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	15	0.29
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	15	0.29
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	15	0.29
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	15	0.29
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	11	0.29
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	11	0.29
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	11	0.29
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	11	0.29
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	11	0.29
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	11	0.29
(1,520)	1:24:A:LEU:HD21	1:23:A:TRP:HZ2	4	0.29
(1,520)	1:24:A:LEU:HD22	1:23:A:TRP:HZ2	4	0.29
(1,520)	1:24:A:LEU:HD23	1:23:A:TRP:HZ2	4	0.29
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	4	0.29
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	4	0.29
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	4	0.29
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	18	0.29
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	18	0.29
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	2	0.29
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	2	0.29
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	2	0.29
(1,40)	1:33:A:LEU:HD21	1:39:A:VAL:H	17	0.29
(1,40)	1:33:A:LEU:HD22	1:39:A:VAL:H	17	0.29
(1,40)	1:33:A:LEU:HD23	1:39:A:VAL:H	17	0.29
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG2	20	0.28
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG3	20	0.28
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	7	0.28
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	7	0.28
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	11	0.28
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	11	0.28
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	11	0.28
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	18	0.28
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	18	0.28
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB1	16	0.28
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB2	16	0.28
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB3	16	0.28
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	18	0.28
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	18	0.28
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	18	0.28
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	1	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	1	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	1	0.28
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	3	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	3	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	3	0.28
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	7	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	7	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	7	0.28
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	9	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	9	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	9	0.28
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	11	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	11	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	11	0.28
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	14	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	14	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	14	0.28
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	17	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	17	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	20	0.28
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	20	0.28
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	20	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	4	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	4	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	4	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	5	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	5	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	5	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	6	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	6	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	6	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	7	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	7	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	7	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	8	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	8	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	8	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	9	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	9	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	9	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	10	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	10	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	10	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	11	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	11	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	11	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	12	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	12	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	12	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	13	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	13	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	13	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	15	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	15	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	15	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	19	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	19	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	19	0.28
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	20	0.28
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	20	0.28
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	1	0.28
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	1	0.28
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	1	0.28
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	1	0.28
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	1	0.28
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	1	0.28
(1,963)	1:92:A:ASN:HA	1:92:A:ASN:HD22	11	0.28
(1,963)	1:92:A:ASN:HA	1:92:A:ASN:HD22	19	0.28
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	4	0.28
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	4	0.28
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	4	0.28
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	15	0.28
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	15	0.28
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	15	0.28
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	18	0.28
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	18	0.28
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	18	0.28
(1,678)	1:48:A:ILE:HD11	1:48:A:ILE:H	18	0.28
(1,678)	1:48:A:ILE:HD12	1:48:A:ILE:H	18	0.28
(1,678)	1:48:A:ILE:HD13	1:48:A:ILE:H	18	0.28
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	11	0.28
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	11	0.28
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	11	0.28
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	19	0.28
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	19	0.28
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	19	0.28
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	19	0.28
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	19	0.28
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	19	0.28
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	5	0.28
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	5	0.28
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	5	0.28
(1,425)	1:62:A:LEU:HD11	1:43:A:LEU:HA	4	0.28
(1,425)	1:62:A:LEU:HD12	1:43:A:LEU:HA	4	0.28
(1,425)	1:62:A:LEU:HD13	1:43:A:LEU:HA	4	0.28
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	16	0.28
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	16	0.28
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	16	0.28
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	9	0.28
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	9	0.28
(1,54)	1:23:A:TRP:H	1:24:A:LEU:H	9	0.28
(1,42)	1:33:A:LEU:HD21	1:27:A:VAL:HG21	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:33:A:LEU:HD21	1:27:A:VAL:HG22	19	0.28
(1,42)	1:33:A:LEU:HD21	1:27:A:VAL:HG23	19	0.28
(1,42)	1:33:A:LEU:HD22	1:27:A:VAL:HG21	19	0.28
(1,42)	1:33:A:LEU:HD22	1:27:A:VAL:HG22	19	0.28
(1,42)	1:33:A:LEU:HD22	1:27:A:VAL:HG23	19	0.28
(1,42)	1:33:A:LEU:HD23	1:27:A:VAL:HG21	19	0.28
(1,42)	1:33:A:LEU:HD23	1:27:A:VAL:HG22	19	0.28
(1,42)	1:33:A:LEU:HD23	1:27:A:VAL:HG23	19	0.28
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	1	0.28
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	1	0.28
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	1	0.28
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	1	0.28
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	1	0.28
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	1	0.28
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	4	0.28
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	4	0.28
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	4	0.28
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD11	16	0.27
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD12	16	0.27
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD13	16	0.27
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	18	0.27
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	18	0.27
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB2	4	0.27
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB3	4	0.27
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	20	0.27
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	20	0.27
(1,1758)	1:54:A:THR:HG21	1:55:A:LEU:H	8	0.27
(1,1758)	1:54:A:THR:HG22	1:55:A:LEU:H	8	0.27
(1,1758)	1:54:A:THR:HG23	1:55:A:LEU:H	8	0.27
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB2	11	0.27
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB3	11	0.27
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	7	0.27
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	7	0.27
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	7	0.27
(1,1621)	1:91:A:GLN:HE21	1:88:A:ARG:HA	10	0.27
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	2	0.27
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	2	0.27
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	2	0.27
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	4	0.27
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	4	0.27
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	4	0.27
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	10	0.27
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	10	0.27
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	1	0.27
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	1	0.27
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	13	0.27
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	13	0.27
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	15	0.27
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	15	0.27
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	16	0.27
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	16	0.27
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	20	0.27
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	20	0.27
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	2	0.27
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	2	0.27
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	2	0.27
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	3	0.27
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	3	0.27
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	3	0.27
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	14	0.27
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	14	0.27
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	14	0.27
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	17	0.27
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	17	0.27
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	17	0.27
(1,1067)	1:105:A:ILE:HG21	1:105:A:ILE:H	18	0.27
(1,1067)	1:105:A:ILE:HG22	1:105:A:ILE:H	18	0.27
(1,1067)	1:105:A:ILE:HG23	1:105:A:ILE:H	18	0.27
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	16	0.27
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	16	0.27
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	16	0.27
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	16	0.27
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	16	0.27
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	16	0.27
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	1	0.27
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	1	0.27
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	1	0.27
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	3	0.27
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	3	0.27
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	3	0.27
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	6	0.27
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	6	0.27
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	12	0.27
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	12	0.27
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	12	0.27
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	14	0.27
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	14	0.27
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	14	0.27
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	17	0.27
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	17	0.27
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	17	0.27
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	9	0.27
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	9	0.27
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	9	0.27
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	10	0.27
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	10	0.27
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE1	2	0.27
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE2	2	0.27
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE1	2	0.27
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE2	2	0.27
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE1	2	0.27
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE2	2	0.27
(1,55)	1:45:A:VAL:HA	1:62:A:LEU:H	4	0.27
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	10	0.27
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	10	0.27
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	10	0.27
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	10	0.27
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	10	0.27
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	10	0.27
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	11	0.27
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	11	0.27
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	11	0.27
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	13	0.26
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	6	0.26
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	6	0.26
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	6	0.26
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	12	0.26
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	12	0.26
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	12	0.26
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	18	0.26
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	18	0.26
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	18	0.26
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB2	6	0.26
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB2	12	0.26
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB3	12	0.26
(1,1853)	1:173:A:GLU:H	1:172:A:GLN:HB2	16	0.26
(1,1853)	1:173:A:GLU:H	1:172:A:GLN:HB3	16	0.26
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG2	4	0.26
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG3	4	0.26
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	9	0.26
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	9	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	3	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	3	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	3	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	6	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	6	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	6	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	8	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	8	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	8	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	9	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	9	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	9	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	10	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	10	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	10	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	11	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	11	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	11	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	12	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	12	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	12	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	15	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	15	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	15	0.26
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	20	0.26
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	20	0.26
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	20	0.26
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD21	10	0.26
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD22	10	0.26
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD23	10	0.26
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	18	0.26
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	18	0.26
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	18	0.26
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG21	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG22	20	0.26
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG23	20	0.26
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG21	20	0.26
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG22	20	0.26
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG23	20	0.26
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	16	0.26
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	16	0.26
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	16	0.26
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD21	6	0.26
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD22	6	0.26
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD23	6	0.26
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD21	12	0.26
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD22	12	0.26
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD23	12	0.26
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	7	0.26
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	7	0.26
(1,1107)	1:113:A:VAL:HG21	1:114:A:GLN:HE22	5	0.26
(1,1107)	1:113:A:VAL:HG22	1:114:A:GLN:HE22	5	0.26
(1,1107)	1:113:A:VAL:HG23	1:114:A:GLN:HE22	5	0.26
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	8	0.26
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	8	0.26
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	8	0.26
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	8	0.26
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	8	0.26
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	8	0.26
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	17	0.26
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	17	0.26
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	17	0.26
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	2	0.26
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	2	0.26
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	2	0.26
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	16	0.26
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	16	0.26
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	16	0.26
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	20	0.26
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	20	0.26
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	20	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	1	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	1	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	1	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	2	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	2	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	4	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	4	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	4	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	5	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	5	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	5	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	6	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	6	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	6	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	7	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	7	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	7	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	10	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	10	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	10	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	11	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	11	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	11	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	12	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	12	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	12	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	16	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	16	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	16	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	17	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	17	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	17	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	19	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	19	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	19	0.26
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	20	0.26
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	20	0.26
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	20	0.26
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	6	0.26
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	6	0.26
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	6	0.26
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	10	0.26
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	10	0.26
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	10	0.26
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	12	0.26
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	12	0.26
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	16	0.26
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	16	0.26
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	16	0.26
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	20	0.26
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	20	0.26
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	20	0.26
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	14	0.26
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	14	0.26
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	14	0.26
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	16	0.26
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	16	0.26
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	16	0.26
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	16	0.26
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	16	0.26
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	16	0.26
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	16	0.26
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	16	0.26
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	16	0.26
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	17	0.26
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	17	0.26
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	17	0.26
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	3	0.26
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	3	0.26
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	3	0.26
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	3	0.26
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	3	0.26
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	3	0.26
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD2	4	0.25
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD3	4	0.25
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	3	0.25
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	3	0.25
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	13	0.25
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	13	0.25
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	13	0.25
(1,1801)	1:41:A:LYS:HD2	1:42:A:VAL:H	9	0.25
(1,1801)	1:41:A:LYS:HD3	1:42:A:VAL:H	9	0.25
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	4	0.25
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	4	0.25
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	4	0.25
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	5	0.25
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	5	0.25
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	13	0.25
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	13	0.25
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	13	0.25
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	14	0.25
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	14	0.25
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	14	0.25
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	17	0.25
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	17	0.25
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	17	0.25
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	10	0.25
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	10	0.25
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	10	0.25
(1,1228)	1:100:A:ILE:HG21	1:137:A:ILE:HD11	16	0.25
(1,1228)	1:100:A:ILE:HG21	1:137:A:ILE:HD12	16	0.25
(1,1228)	1:100:A:ILE:HG21	1:137:A:ILE:HD13	16	0.25
(1,1228)	1:100:A:ILE:HG22	1:137:A:ILE:HD11	16	0.25
(1,1228)	1:100:A:ILE:HG22	1:137:A:ILE:HD12	16	0.25
(1,1228)	1:100:A:ILE:HG22	1:137:A:ILE:HD13	16	0.25
(1,1228)	1:100:A:ILE:HG23	1:137:A:ILE:HD11	16	0.25
(1,1228)	1:100:A:ILE:HG23	1:137:A:ILE:HD12	16	0.25
(1,1228)	1:100:A:ILE:HG23	1:137:A:ILE:HD13	16	0.25
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD21	5	0.25
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD22	5	0.25
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD23	5	0.25
(1,948)	1:89:A:VAL:HG21	1:89:A:VAL:H	7	0.25
(1,948)	1:89:A:VAL:HG22	1:89:A:VAL:H	7	0.25
(1,948)	1:89:A:VAL:HG23	1:89:A:VAL:H	7	0.25
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	3	0.25
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	3	0.25
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	3	0.25
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	8	0.25
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	8	0.25
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	8	0.25
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	9	0.25
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	9	0.25
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	9	0.25
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	13	0.25
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	13	0.25
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	13	0.25
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	14	0.25
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	14	0.25
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	15	0.25
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	15	0.25
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	15	0.25
(1,900)	1:78:A:ILE:HG21	1:78:A:ILE:H	18	0.25
(1,900)	1:78:A:ILE:HG22	1:78:A:ILE:H	18	0.25
(1,900)	1:78:A:ILE:HG23	1:78:A:ILE:H	18	0.25
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	2	0.25
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	2	0.25
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	2	0.25
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	2	0.25
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	2	0.25
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	2	0.25
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	2	0.25
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	2	0.25
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	2	0.25
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	10	0.25
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	10	0.25
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	10	0.25
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	14	0.25
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	14	0.25
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	14	0.25
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	8	0.25
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	8	0.25
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	8	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	3	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	3	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	3	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	4	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	4	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	4	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	7	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	7	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	7	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	13	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	13	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	13	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	15	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	15	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	15	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	17	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	17	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	18	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	18	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	18	0.25
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	19	0.25
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	19	0.25
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	19	0.25
(1,205)	1:75:A:TYR:HE1	1:55:A:LEU:HD21	14	0.25
(1,205)	1:75:A:TYR:HE1	1:55:A:LEU:HD22	14	0.25
(1,205)	1:75:A:TYR:HE1	1:55:A:LEU:HD23	14	0.25
(1,205)	1:75:A:TYR:HE2	1:55:A:LEU:HD21	14	0.25
(1,205)	1:75:A:TYR:HE2	1:55:A:LEU:HD22	14	0.25
(1,205)	1:75:A:TYR:HE2	1:55:A:LEU:HD23	14	0.25
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	7	0.25
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	7	0.25
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	18	0.25
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	18	0.25
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	13	0.25
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	13	0.25
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	13	0.25
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	8	0.25
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	8	0.25
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	8	0.25
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	8	0.25
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	8	0.25
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	8	0.25
(1,8)	1:96:A:SER:HA	1:147:A:GLN:HG2	16	0.25
(1,8)	1:96:A:SER:HA	1:147:A:GLN:HG3	16	0.25
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	1	0.24
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	1	0.24
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	1	0.24
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	8	0.24
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	8	0.24
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	8	0.24
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	17	0.24
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	17	0.24
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	17	0.24
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	3	0.24
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	3	0.24
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB1	8	0.24
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB2	8	0.24
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB3	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	17	0.24
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB2	19	0.24
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB3	19	0.24
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	6	0.24
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	12	0.24
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	11	0.24
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	11	0.24
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	11	0.24
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD21	16	0.24
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD22	16	0.24
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD23	16	0.24
(1,700)	1:55:A:LEU:HD11	1:55:A:LEU:H	10	0.24
(1,700)	1:55:A:LEU:HD12	1:55:A:LEU:H	10	0.24
(1,700)	1:55:A:LEU:HD13	1:55:A:LEU:H	10	0.24
(1,678)	1:48:A:ILE:HD11	1:48:A:ILE:H	4	0.24
(1,678)	1:48:A:ILE:HD12	1:48:A:ILE:H	4	0.24
(1,678)	1:48:A:ILE:HD13	1:48:A:ILE:H	4	0.24
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	1	0.24
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	1	0.24
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	1	0.24
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	1	0.24
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	1	0.24
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	1	0.24
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	1	0.24
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	1	0.24
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	1	0.24
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	2	0.24
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	2	0.24
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	2	0.24
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	8	0.24
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	8	0.24
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	8	0.24
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	9	0.24
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	9	0.24
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	9	0.24
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	11	0.24
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	11	0.24
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	11	0.24
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	1	0.24
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	1	0.24
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	1	0.24
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	17	0.24
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	17	0.24
(1,425)	1:62:A:LEU:HD11	1:43:A:LEU:HA	9	0.24
(1,425)	1:62:A:LEU:HD12	1:43:A:LEU:HA	9	0.24
(1,425)	1:62:A:LEU:HD13	1:43:A:LEU:HA	9	0.24
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	6	0.24
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	6	0.24
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	6	0.24
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	6	0.24
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	6	0.24
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	6	0.24
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	6	0.24
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	6	0.24
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	6	0.24
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	12	0.24
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	12	0.24
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	12	0.24
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	12	0.24
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	12	0.24
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	12	0.24
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	12	0.24
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	12	0.24
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	12	0.24
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	8	0.24
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	8	0.24
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	8	0.24
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	15	0.24
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	15	0.24
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	15	0.24
(1,288)	1:31:A:ALA:HB1	1:33:A:LEU:HB2	17	0.24
(1,288)	1:31:A:ALA:HB1	1:33:A:LEU:HB3	17	0.24
(1,288)	1:31:A:ALA:HB2	1:33:A:LEU:HB2	17	0.24
(1,288)	1:31:A:ALA:HB2	1:33:A:LEU:HB3	17	0.24
(1,288)	1:31:A:ALA:HB3	1:33:A:LEU:HB2	17	0.24
(1,288)	1:31:A:ALA:HB3	1:33:A:LEU:HB3	17	0.24
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB2	14	0.24
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB3	14	0.24
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB2	14	0.24
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB3	14	0.24
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE2	8	0.24
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE3	8	0.24
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE2	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE3	8	0.24
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	6	0.24
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	6	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	6	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	6	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	6	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	6	0.24
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	12	0.24
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	12	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	12	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	12	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	12	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	12	0.24
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	20	0.24
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	20	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	20	0.24
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	20	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	20	0.24
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	20	0.24
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG21	15	0.24
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG22	15	0.24
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG23	15	0.24
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG21	15	0.24
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG22	15	0.24
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG23	15	0.24
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG21	15	0.24
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG22	15	0.24
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG23	15	0.24
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	7	0.24
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	7	0.24
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	7	0.24
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	19	0.24
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	19	0.24
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	19	0.24
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	7	0.24
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	7	0.24
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	7	0.24
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	7	0.24
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	7	0.24
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	7	0.24
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD11	13	0.23
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD12	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD13	13	0.23
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	1	0.23
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	1	0.23
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	1	0.23
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	15	0.23
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	17	0.23
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	14	0.23
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	14	0.23
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	3	0.23
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	3	0.23
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	3	0.23
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	5	0.23
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	5	0.23
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	5	0.23
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB2	11	0.23
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB3	11	0.23
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD11	4	0.23
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD12	4	0.23
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD13	4	0.23
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	13	0.23
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	13	0.23
(1,1779)	1:20:A:MET:H	1:20:A:MET:HG2	7	0.23
(1,1779)	1:20:A:MET:H	1:20:A:MET:HG3	7	0.23
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB1	9	0.23
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB2	9	0.23
(1,1769)	1:11:A:ALA:H	1:11:A:ALA:HB3	9	0.23
(1,1736)	1:29:A:CYS:H	1:30:A:GLU:HA	10	0.23
(1,1678)	1:170:A:ILE:HG21	1:170:A:ILE:H	16	0.23
(1,1678)	1:170:A:ILE:HG22	1:170:A:ILE:H	16	0.23
(1,1678)	1:170:A:ILE:HG23	1:170:A:ILE:H	16	0.23
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	3	0.23
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	3	0.23
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	3	0.23
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	6	0.23
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	6	0.23
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	6	0.23
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	9	0.23
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	9	0.23
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	9	0.23
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	12	0.23
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	12	0.23
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	20	0.23
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	20	0.23
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	20	0.23
(1,1350)	1:159:A:LEU:HD21	1:160:A:TYR:HB2	9	0.23
(1,1350)	1:159:A:LEU:HD21	1:160:A:TYR:HB3	9	0.23
(1,1350)	1:159:A:LEU:HD22	1:160:A:TYR:HB2	9	0.23
(1,1350)	1:159:A:LEU:HD22	1:160:A:TYR:HB3	9	0.23
(1,1350)	1:159:A:LEU:HD23	1:160:A:TYR:HB2	9	0.23
(1,1350)	1:159:A:LEU:HD23	1:160:A:TYR:HB3	9	0.23
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	5	0.23
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	5	0.23
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	8	0.23
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	8	0.23
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	19	0.23
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	19	0.23
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	13	0.23
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	13	0.23
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	13	0.23
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	13	0.23
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	13	0.23
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	13	0.23
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	10	0.23
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	10	0.23
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	10	0.23
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	10	0.23
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	10	0.23
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	10	0.23
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	4	0.23
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	4	0.23
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	4	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	3	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	3	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	3	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	6	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	6	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	6	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	9	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	9	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	9	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	10	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	10	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	12	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	12	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	12	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	13	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	13	0.23
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	13	0.23
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	5	0.23
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	5	0.23
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	5	0.23
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	10	0.23
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	10	0.23
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	10	0.23
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	6	0.23
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	6	0.23
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	6	0.23
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	8	0.23
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	8	0.23
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	8	0.23
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	12	0.23
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	12	0.23
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	12	0.23
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	13	0.23
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	13	0.23
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	13	0.23
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	10	0.23
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	10	0.23
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	10	0.23
(1,578)	1:34:A:GLY:HA2	1:36:A:ASN:H	17	0.23
(1,578)	1:34:A:GLY:HA3	1:36:A:ASN:H	17	0.23
(1,506)	1:23:A:TRP:HD1	1:23:A:TRP:HA	13	0.23
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	7	0.23
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	7	0.23
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	7	0.23
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	6	0.23
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	6	0.23
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	12	0.23
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	12	0.23
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD1	17	0.23
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD2	17	0.23
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD1	17	0.23
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD2	17	0.23
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:39:A:VAL:HG21	1:40:A:ASP:HA	19	0.23
(1,284)	1:39:A:VAL:HG22	1:40:A:ASP:HA	19	0.23
(1,284)	1:39:A:VAL:HG23	1:40:A:ASP:HA	19	0.23
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	10	0.23
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	10	0.23
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	10	0.23
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD1	13	0.23
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD2	13	0.23
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	10	0.22
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	10	0.22
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	10	0.22
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	11	0.22
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	11	0.22
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	11	0.22
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB2	14	0.22
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB3	14	0.22
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	3	0.22
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	3	0.22
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG21	18	0.22
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG22	18	0.22
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG23	18	0.22
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	1	0.22
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	1	0.22
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	4	0.22
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	4	0.22
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	4	0.22
(1,1933)	1:176:A:ASP:H	1:175:A:SER:HB2	16	0.22
(1,1933)	1:176:A:ASP:H	1:175:A:SER:HB3	16	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	14	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	14	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	14	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	16	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	16	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	16	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	18	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	18	0.22
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	18	0.22
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	9	0.22
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	9	0.22
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	10	0.22
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	10	0.22
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	2	0.22
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	2	0.22
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	11	0.22
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	11	0.22
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	11	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	2	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	2	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	2	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	7	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	7	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	7	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	14	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	14	0.22
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	14	0.22
(1,1477)	1:114:A:GLN:HE22	1:114:A:GLN:HB2	5	0.22
(1,1477)	1:114:A:GLN:HE22	1:114:A:GLN:HB3	5	0.22
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	2	0.22
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	2	0.22
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	2	0.22
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	8	0.22
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	8	0.22
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	8	0.22
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	11	0.22
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	11	0.22
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	11	0.22
(1,1416)	1:170:A:ILE:HD11	1:170:A:ILE:HB	19	0.22
(1,1416)	1:170:A:ILE:HD12	1:170:A:ILE:HB	19	0.22
(1,1416)	1:170:A:ILE:HD13	1:170:A:ILE:HB	19	0.22
(1,1313)	1:156:A:ILE:HD11	1:156:A:ILE:HA	5	0.22
(1,1313)	1:156:A:ILE:HD12	1:156:A:ILE:HA	5	0.22
(1,1313)	1:156:A:ILE:HD13	1:156:A:ILE:HA	5	0.22
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	2	0.22
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	2	0.22
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	2	0.22
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	4	0.22
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	4	0.22
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	4	0.22
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	6	0.22
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	6	0.22
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	6	0.22
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	12	0.22
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	12	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD11	8	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD12	8	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD13	8	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD11	10	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD12	10	0.22
(1,1280)	1:149:A:ILE:HB	1:149:A:ILE:HD13	10	0.22
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	5	0.22
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	5	0.22
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	5	0.22
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	5	0.22
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	5	0.22
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	5	0.22
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	1	0.22
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	1	0.22
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	1	0.22
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	1	0.22
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	1	0.22
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	1	0.22
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	1	0.22
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	1	0.22
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	1	0.22
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	13	0.22
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	13	0.22
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	20	0.22
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	20	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	9	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	9	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	9	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	10	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	10	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	10	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	11	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	11	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	11	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	13	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	13	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	13	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	14	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	14	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	14	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	15	0.22
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	15	0.22
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	7	0.22
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	7	0.22
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	7	0.22
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	7	0.22
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	7	0.22
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	7	0.22
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	7	0.22
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	7	0.22
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	7	0.22
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	16	0.22
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	16	0.22
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	16	0.22
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	16	0.22
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	16	0.22
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	16	0.22
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	16	0.22
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	16	0.22
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	16	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	1	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	1	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	1	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	2	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	2	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	2	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	3	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	3	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	3	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	5	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	5	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	5	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	6	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	6	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	6	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	7	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	7	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	7	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	8	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	8	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	8	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	9	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	9	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	10	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	10	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	10	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	11	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	11	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	11	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	12	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	12	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	12	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	13	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	13	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	13	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	14	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	14	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	14	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	15	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	15	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	15	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	16	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	16	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	16	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	17	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	17	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	17	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	18	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	18	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	18	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	19	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	19	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	19	0.22
(1,795)	1:69:A:ILE:HD11	1:69:A:ILE:HB	20	0.22
(1,795)	1:69:A:ILE:HD12	1:69:A:ILE:HB	20	0.22
(1,795)	1:69:A:ILE:HD13	1:69:A:ILE:HB	20	0.22
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	9	0.22
(1,703)	1:55:A:LEU:HG	1:55:A:LEU:H	2	0.22
(1,700)	1:55:A:LEU:HD11	1:55:A:LEU:H	2	0.22
(1,700)	1:55:A:LEU:HD12	1:55:A:LEU:H	2	0.22
(1,700)	1:55:A:LEU:HD13	1:55:A:LEU:H	2	0.22
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	4	0.22
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	4	0.22
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	18	0.22
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	18	0.22
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	18	0.22
(1,615)	1:41:A:LYS:HD2	1:41:A:LYS:HA	19	0.22
(1,615)	1:41:A:LYS:HD3	1:41:A:LYS:HA	19	0.22
(1,614)	1:41:A:LYS:HA	1:41:A:LYS:HD2	19	0.22
(1,614)	1:41:A:LYS:HA	1:41:A:LYS:HD3	19	0.22
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD1	14	0.22
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD2	14	0.22
(1,578)	1:34:A:GLY:HA2	1:36:A:ASN:H	7	0.22
(1,578)	1:34:A:GLY:HA3	1:36:A:ASN:H	7	0.22
(1,578)	1:34:A:GLY:HA2	1:36:A:ASN:H	13	0.22
(1,578)	1:34:A:GLY:HA3	1:36:A:ASN:H	13	0.22
(1,573)	1:33:A:LEU:HD11	1:33:A:LEU:H	11	0.22
(1,573)	1:33:A:LEU:HD12	1:33:A:LEU:H	11	0.22
(1,573)	1:33:A:LEU:HD13	1:33:A:LEU:H	11	0.22
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	5	0.22
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	5	0.22
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	5	0.22
(1,462)	1:8:A:SER:HB2	1:10:A:ASP:H	20	0.22
(1,462)	1:8:A:SER:HB3	1:10:A:ASP:H	20	0.22
(1,409)	1:171:A:GLU:HB2	1:172:A:GLN:H	5	0.22
(1,409)	1:171:A:GLU:HB3	1:172:A:GLN:H	5	0.22
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	18	0.22
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	18	0.22
(1,374)	1:62:A:LEU:HD21	1:69:A:ILE:H	5	0.22
(1,374)	1:62:A:LEU:HD22	1:69:A:ILE:H	5	0.22
(1,374)	1:62:A:LEU:HD23	1:69:A:ILE:H	5	0.22
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	11	0.22
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	11	0.22
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	11	0.22
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	11	0.22
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	11	0.22
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	11	0.22
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	11	0.22
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	11	0.22
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	11	0.22
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	17	0.22
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	17	0.22
(1,302)	1:15:A:THR:HG21	1:15:A:THR:HA	5	0.22
(1,302)	1:15:A:THR:HG22	1:15:A:THR:HA	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:15:A:THR:HG23	1:15:A:THR:HA	5	0.22
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	16	0.22
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	16	0.22
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	16	0.22
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB2	3	0.22
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB3	3	0.22
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB2	3	0.22
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB3	3	0.22
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB2	3	0.22
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB3	3	0.22
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB2	11	0.22
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB3	11	0.22
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB2	11	0.22
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB3	11	0.22
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB2	11	0.22
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB3	11	0.22
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD1	18	0.22
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD2	18	0.22
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	4	0.22
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	4	0.22
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	4	0.22
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	17	0.22
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	17	0.22
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	17	0.22
(1,161)	1:156:A:ILE:HG21	1:63:A:CYS:HB2	5	0.22
(1,161)	1:156:A:ILE:HG21	1:63:A:CYS:HB3	5	0.22
(1,161)	1:156:A:ILE:HG22	1:63:A:CYS:HB2	5	0.22
(1,161)	1:156:A:ILE:HG22	1:63:A:CYS:HB3	5	0.22
(1,161)	1:156:A:ILE:HG23	1:63:A:CYS:HB2	5	0.22
(1,161)	1:156:A:ILE:HG23	1:63:A:CYS:HB3	5	0.22
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	5	0.22
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	5	0.22
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	5	0.22
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	18	0.22
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	18	0.22
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	18	0.22
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD2	18	0.22
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD3	18	0.22
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	3	0.22
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	3	0.22
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	3	0.22
(1,55)	1:45:A:VAL:HA	1:62:A:LEU:H	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG21	5	0.22
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG22	5	0.22
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG23	5	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG21	5	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG22	5	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG23	5	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG21	5	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG22	5	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG23	5	0.22
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG21	11	0.22
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG22	11	0.22
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG23	11	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG21	11	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG22	11	0.22
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG23	11	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG21	11	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG22	11	0.22
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG23	11	0.22
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	17	0.22
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	17	0.22
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	17	0.22
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	9	0.21
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	9	0.21
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	9	0.21
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	1	0.21
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	7	0.21
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	7	0.21
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	9	0.21
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	9	0.21
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	19	0.21
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	19	0.21
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	3	0.21
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	3	0.21
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	3	0.21
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB2	11	0.21
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB3	11	0.21
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD11	15	0.21
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD12	15	0.21
(1,1809)	1:129:A:PHE:H	1:128:A:LEU:HD13	15	0.21
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	10	0.21
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	10	0.21
(1,1736)	1:29:A:CYS:H	1:30:A:GLU:HA	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	10	0.21
(1,1497)	1:161:A:GLY:H	1:160:A:TYR:HD1	1	0.21
(1,1497)	1:161:A:GLY:H	1:160:A:TYR:HD2	1	0.21
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD11	9	0.21
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD12	9	0.21
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD13	9	0.21
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	10	0.21
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	10	0.21
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	10	0.21
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	19	0.21
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	19	0.21
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	19	0.21
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	10	0.21
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	10	0.21
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	17	0.21
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	17	0.21
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	11	0.21
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	11	0.21
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	11	0.21
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	11	0.21
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	11	0.21
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	11	0.21
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	11	0.21
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	11	0.21
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	11	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	1	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	1	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	4	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	4	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	6	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	6	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	12	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	12	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD1	18	0.21
(1,1074)	1:107:A:PHE:HA	1:107:A:PHE:HD2	18	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	1	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	1	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	1	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	2	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	2	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	2	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	3	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	3	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	4	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	4	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	4	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	5	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	5	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	5	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	6	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	6	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	6	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	7	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	7	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	7	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	8	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	8	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	8	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	12	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	12	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	12	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	16	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	16	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	16	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	17	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	17	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	17	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	18	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	18	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	18	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	19	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	19	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	19	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD11	20	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD12	20	0.21
(1,1063)	1:105:A:ILE:HB	1:105:A:ILE:HD13	20	0.21
(1,1016)	1:99:A:MET:HE1	1:143:A:PHE:HZ	10	0.21
(1,1016)	1:99:A:MET:HE2	1:143:A:PHE:HZ	10	0.21
(1,1016)	1:99:A:MET:HE3	1:143:A:PHE:HZ	10	0.21
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	19	0.21
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	19	0.21
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	19	0.21
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	19	0.21
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	19	0.21
(1,958)	1:90:A:THR:HB	1:91:A:GLN:H	15	0.21
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	4	0.21
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	4	0.21
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	4	0.21
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	4	0.21
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	4	0.21
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	4	0.21
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	4	0.21
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	4	0.21
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	4	0.21
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD21	2	0.21
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD22	2	0.21
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD23	2	0.21
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD21	2	0.21
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD22	2	0.21
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD23	2	0.21
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD21	2	0.21
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD22	2	0.21
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD23	2	0.21
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD21	11	0.21
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD22	11	0.21
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD23	11	0.21
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD21	11	0.21
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD22	11	0.21
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD23	11	0.21
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD21	11	0.21
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD22	11	0.21
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD23	11	0.21
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	2	0.21
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	2	0.21
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	2	0.21
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG21	20	0.21
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG22	20	0.21
(1,695)	1:54:A:THR:HA	1:54:A:THR:HG23	20	0.21
(1,678)	1:48:A:ILE:HD11	1:48:A:ILE:H	9	0.21
(1,678)	1:48:A:ILE:HD12	1:48:A:ILE:H	9	0.21
(1,678)	1:48:A:ILE:HD13	1:48:A:ILE:H	9	0.21
(1,676)	1:48:A:ILE:HB	1:48:A:ILE:H	16	0.21
(1,669)	1:47:A:ARG:HD2	1:48:A:ILE:H	2	0.21
(1,669)	1:47:A:ARG:HD3	1:48:A:ILE:H	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	1	0.21
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	1	0.21
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	1	0.21
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	6	0.21
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	6	0.21
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	6	0.21
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	12	0.21
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	12	0.21
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	12	0.21
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	4	0.21
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	4	0.21
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	4	0.21
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	4	0.21
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	4	0.21
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	4	0.21
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	20	0.21
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	20	0.21
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	20	0.21
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD1	11	0.21
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD2	11	0.21
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	3	0.21
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	3	0.21
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	3	0.21
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	2	0.21
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	2	0.21
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	19	0.21
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	19	0.21
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	10	0.21
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	10	0.21
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	10	0.21
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	14	0.21
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	14	0.21
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	14	0.21
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	17	0.21
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	17	0.21
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	17	0.21
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	19	0.21
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	19	0.21
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	19	0.21
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	5	0.21
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	5	0.21
(1,302)	1:15:A:THR:HG21	1:15:A:THR:HA	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:15:A:THR:HG22	1:15:A:THR:HA	3	0.21
(1,302)	1:15:A:THR:HG23	1:15:A:THR:HA	3	0.21
(1,302)	1:15:A:THR:HG21	1:15:A:THR:HA	7	0.21
(1,302)	1:15:A:THR:HG22	1:15:A:THR:HA	7	0.21
(1,302)	1:15:A:THR:HG23	1:15:A:THR:HA	7	0.21
(1,302)	1:15:A:THR:HG21	1:15:A:THR:HA	18	0.21
(1,302)	1:15:A:THR:HG22	1:15:A:THR:HA	18	0.21
(1,302)	1:15:A:THR:HG23	1:15:A:THR:HA	18	0.21
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	2	0.21
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	2	0.21
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	2	0.21
(1,183)	1:135:A:LEU:HD21	1:23:A:TRP:HH2	2	0.21
(1,183)	1:135:A:LEU:HD22	1:23:A:TRP:HH2	2	0.21
(1,183)	1:135:A:LEU:HD23	1:23:A:TRP:HH2	2	0.21
(1,183)	1:135:A:LEU:HD21	1:23:A:TRP:HH2	20	0.21
(1,183)	1:135:A:LEU:HD22	1:23:A:TRP:HH2	20	0.21
(1,183)	1:135:A:LEU:HD23	1:23:A:TRP:HH2	20	0.21
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG21	19	0.21
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG22	19	0.21
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG23	19	0.21
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG21	19	0.21
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG22	19	0.21
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG23	19	0.21
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG21	19	0.21
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG22	19	0.21
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG23	19	0.21
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	15	0.21
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	15	0.21
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	15	0.21
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD1	14	0.21
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD2	14	0.21
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD1	14	0.21
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD2	14	0.21
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD1	14	0.21
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD2	14	0.21
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	2	0.21
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	2	0.21
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	2	0.21
(1,2225)	1:98:A:ILE:H	1:44:A:LYS:HA	20	0.2
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG2	3	0.2
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG3	3	0.2
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG2	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG3	17	0.2
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	17	0.2
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	17	0.2
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	17	0.2
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	5	0.2
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	5	0.2
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	5	0.2
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	5	0.2
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	7	0.2
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	8	0.2
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	15	0.2
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	4	0.2
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	4	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	2	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	2	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	2	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	7	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	7	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	7	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	8	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	8	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	8	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	10	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	10	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	10	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	20	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	20	0.2
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	20	0.2
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	11	0.2
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	11	0.2
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	11	0.2
(1,1808)	1:129:A:PHE:H	1:128:A:LEU:HB2	14	0.2
(1,1808)	1:129:A:PHE:H	1:128:A:LEU:HB3	14	0.2
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	14	0.2
(1,1736)	1:29:A:CYS:H	1:30:A:GLU:HA	20	0.2
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD11	20	0.2
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD12	20	0.2
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD13	20	0.2
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	11	0.2
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	11	0.2
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	11	0.2
(1,1547)	1:168:A:ARG:H	1:169:A:PHE:HD1	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:168:A:ARG:H	1:169:A:PHE:HD2	3	0.2
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	16	0.2
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	16	0.2
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	16	0.2
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	17	0.2
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	17	0.2
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	17	0.2
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	8	0.2
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	8	0.2
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	8	0.2
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	8	0.2
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	8	0.2
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	8	0.2
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	17	0.2
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	17	0.2
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	17	0.2
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	17	0.2
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	17	0.2
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	17	0.2
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	17	0.2
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	17	0.2
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	17	0.2
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	11	0.2
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	11	0.2
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	11	0.2
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	20	0.2
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	20	0.2
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	20	0.2
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	20	0.2
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	20	0.2
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	20	0.2
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	20	0.2
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	20	0.2
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	20	0.2
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	19	0.2
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	19	0.2
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	19	0.2
(1,676)	1:48:A:ILE:HB	1:48:A:ILE:H	14	0.2
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	15	0.2
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	15	0.2
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	15	0.2
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	20	0.2
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	20	0.2
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	4	0.2
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	4	0.2
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	4	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	1	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	1	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	1	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	3	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	3	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	3	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	4	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	4	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	4	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	5	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	5	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	5	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	6	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	6	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	6	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	8	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	8	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	8	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	10	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	10	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	10	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	11	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	11	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	11	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	12	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	12	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	12	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	14	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	14	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	14	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	15	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	15	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	15	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	16	0.2
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	16	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	16	0.2
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	17	0.2
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	17	0.2
(1,542)	1:27:A:VAL:HG21	1:27:A:VAL:H	14	0.2
(1,542)	1:27:A:VAL:HG22	1:27:A:VAL:H	14	0.2
(1,542)	1:27:A:VAL:HG23	1:27:A:VAL:H	14	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	13	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	13	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	13	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	16	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	16	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	16	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	17	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	17	0.2
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	17	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	1	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	1	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	1	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	3	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	3	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	3	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	7	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	7	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	7	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	8	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	8	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	8	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	9	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	9	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	9	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	10	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	10	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	10	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	11	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	11	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	11	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	13	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	13	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	13	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	16	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	16	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	16	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	17	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	17	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	18	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	18	0.2
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	18	0.2
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	17	0.2
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	17	0.2
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	17	0.2
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG21	14	0.2
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG22	14	0.2
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG23	14	0.2
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG21	14	0.2
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG22	14	0.2
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG23	14	0.2
(1,409)	1:171:A:GLU:HB2	1:172:A:GLN:H	6	0.2
(1,409)	1:171:A:GLU:HB3	1:172:A:GLN:H	6	0.2
(1,409)	1:171:A:GLU:HB2	1:172:A:GLN:H	12	0.2
(1,409)	1:171:A:GLU:HB3	1:172:A:GLN:H	12	0.2
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	5	0.2
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	5	0.2
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	5	0.2
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	5	0.2
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	5	0.2
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	5	0.2
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	5	0.2
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	5	0.2
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	5	0.2
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	17	0.2
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	17	0.2
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	17	0.2
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	19	0.2
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	19	0.2
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	1	0.2
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	1	0.2
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	1	0.2
(1,136)	1:76:A:LYS:HB2	1:74:A:ASN:HD21	17	0.2
(1,136)	1:76:A:LYS:HB2	1:74:A:ASN:HD22	17	0.2
(1,136)	1:76:A:LYS:HB3	1:74:A:ASN:HD21	17	0.2
(1,136)	1:76:A:LYS:HB3	1:74:A:ASN:HD22	17	0.2
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	18	0.2
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	18	0.2
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	9	0.2
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	9	0.2
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	9	0.2
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	9	0.2
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	9	0.2
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	9	0.2
(1,28)	1:105:A:ILE:HG12	1:169:A:PHE:HE1	2	0.2
(1,28)	1:105:A:ILE:HG12	1:169:A:PHE:HE2	2	0.2
(1,28)	1:105:A:ILE:HG13	1:169:A:PHE:HE1	2	0.2
(1,28)	1:105:A:ILE:HG13	1:169:A:PHE:HE2	2	0.2
(1,13)	1:142:A:MET:HE1	1:94:A:LEU:HG	6	0.2
(1,13)	1:142:A:MET:HE2	1:94:A:LEU:HG	6	0.2
(1,13)	1:142:A:MET:HE3	1:94:A:LEU:HG	6	0.2
(1,13)	1:142:A:MET:HE1	1:94:A:LEU:HG	12	0.2
(1,13)	1:142:A:MET:HE2	1:94:A:LEU:HG	12	0.2
(1,13)	1:142:A:MET:HE3	1:94:A:LEU:HG	12	0.2
(1,2214)	1:100:A:ILE:H	1:42:A:VAL:HA	9	0.19
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	3	0.19
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	3	0.19
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	3	0.19
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	14	0.19
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	14	0.19
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	14	0.19
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB1	10	0.19
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB2	10	0.19
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB3	10	0.19
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	2	0.19
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	2	0.19
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	2	0.19
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	19	0.19
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	19	0.19
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	19	0.19
(1,2179)	1:142:A:MET:H	1:84:A:LYS:HB2	1	0.19
(1,2179)	1:142:A:MET:H	1:84:A:LYS:HB3	1	0.19
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	15	0.19
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	15	0.19
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	15	0.19
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	5	0.19
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	11	0.19
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	11	0.19
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE1	3	0.19
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE2	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	8	0.19
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	8	0.19
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	11	0.19
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	11	0.19
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	2	0.19
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	2	0.19
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	13	0.19
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	13	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	1	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	1	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	1	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	9	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	9	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	9	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	15	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	15	0.19
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	15	0.19
(1,1853)	1:173:A:GLU:H	1:172:A:GLN:HB2	11	0.19
(1,1853)	1:173:A:GLU:H	1:172:A:GLN:HB3	11	0.19
(1,1779)	1:20:A:MET:H	1:20:A:MET:HG2	20	0.19
(1,1779)	1:20:A:MET:H	1:20:A:MET:HG3	20	0.19
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD11	16	0.19
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD12	16	0.19
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD13	16	0.19
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	3	0.19
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	8	0.19
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	8	0.19
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	17	0.19
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	17	0.19
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	17	0.19
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	1	0.19
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	16	0.19
(1,1482)	1:121:A:LYS:HE2	1:114:A:GLN:HE22	9	0.19
(1,1482)	1:121:A:LYS:HE3	1:114:A:GLN:HE22	9	0.19
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG21	5	0.19
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG22	5	0.19
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG23	5	0.19
(1,1312)	1:156:A:ILE:HD11	1:156:A:ILE:H	5	0.19
(1,1312)	1:156:A:ILE:HD12	1:156:A:ILE:H	5	0.19
(1,1312)	1:156:A:ILE:HD13	1:156:A:ILE:H	5	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD21	6	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD22	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD23	6	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD21	12	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD22	12	0.19
(1,1273)	1:148:A:LEU:HA	1:148:A:LEU:HD23	12	0.19
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	4	0.19
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	4	0.19
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	11	0.19
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	11	0.19
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	11	0.19
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	11	0.19
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	11	0.19
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	11	0.19
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	11	0.19
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	11	0.19
(1,850)	1:73:A:ALA:HB1	1:137:A:ILE:H	16	0.19
(1,850)	1:73:A:ALA:HB2	1:137:A:ILE:H	16	0.19
(1,850)	1:73:A:ALA:HB3	1:137:A:ILE:H	16	0.19
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	15	0.19
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	15	0.19
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	15	0.19
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	15	0.19
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	15	0.19
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	15	0.19
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	15	0.19
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	15	0.19
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	15	0.19
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	13	0.19
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	13	0.19
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	13	0.19
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	13	0.19
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	13	0.19
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	13	0.19
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	13	0.19
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	13	0.19
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	13	0.19
(1,700)	1:55:A:LEU:HD11	1:55:A:LEU:H	6	0.19
(1,700)	1:55:A:LEU:HD12	1:55:A:LEU:H	6	0.19
(1,700)	1:55:A:LEU:HD13	1:55:A:LEU:H	6	0.19
(1,700)	1:55:A:LEU:HD11	1:55:A:LEU:H	12	0.19
(1,700)	1:55:A:LEU:HD12	1:55:A:LEU:H	12	0.19
(1,700)	1:55:A:LEU:HD13	1:55:A:LEU:H	12	0.19
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD21	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD22	20	0.19
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD23	20	0.19
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD21	20	0.19
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD22	20	0.19
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD23	20	0.19
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD21	20	0.19
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD22	20	0.19
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD23	20	0.19
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG2	5	0.19
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG3	5	0.19
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	3	0.19
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	3	0.19
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	3	0.19
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	15	0.19
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	15	0.19
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	15	0.19
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	11	0.19
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	11	0.19
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	11	0.19
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	1	0.19
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	1	0.19
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	1	0.19
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	13	0.19
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	13	0.19
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	13	0.19
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	13	0.19
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	13	0.19
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	13	0.19
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	2	0.19
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	2	0.19
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	2	0.19
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	7	0.19
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	7	0.19
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	7	0.19
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	9	0.19
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	9	0.19
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	9	0.19
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	13	0.19
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	13	0.19
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	13	0.19
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	18	0.19
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	18	0.19
(1,606)	1:39:A:VAL:HG21	1:39:A:VAL:HA	19	0.19
(1,606)	1:39:A:VAL:HG22	1:39:A:VAL:HA	19	0.19
(1,606)	1:39:A:VAL:HG23	1:39:A:VAL:HA	19	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	1	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	1	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	1	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	2	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	2	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	2	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	4	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	4	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	4	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	5	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	5	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	5	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	6	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	6	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	6	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	8	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	8	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	8	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	9	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	9	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	9	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	10	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	10	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	10	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	11	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	11	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	11	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	12	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	12	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	12	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	14	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	14	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	14	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	15	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	15	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	15	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	19	0.19
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	19	0.19
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	18	0.19
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	18	0.19
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	18	0.19
(1,506)	1:23:A:TRP:HD1	1:23:A:TRP:HA	14	0.19
(1,499)	1:20:A:MET:HE1	1:65:A:ALA:HA	7	0.19
(1,499)	1:20:A:MET:HE2	1:65:A:ALA:HA	7	0.19
(1,499)	1:20:A:MET:HE3	1:65:A:ALA:HA	7	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	2	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	2	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	2	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	4	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	4	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	4	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	5	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	5	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	5	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	6	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	6	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	6	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	12	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	12	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	12	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	14	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	14	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	14	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	19	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	19	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	19	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	20	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	20	0.19
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	20	0.19
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	5	0.19
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	5	0.19
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	5	0.19
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	20	0.19
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	20	0.19
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	20	0.19
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	1	0.19
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	1	0.19
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	1	0.19
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	1	0.19
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	1	0.19
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	4	0.19
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	4	0.19
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	6	0.19
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	6	0.19
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	6	0.19
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	12	0.19
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	12	0.19
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	12	0.19
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	15	0.19
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	15	0.19
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	15	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	2	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	2	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	2	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	2	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	2	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	2	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	2	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	2	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	2	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	17	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	17	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	17	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	17	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	17	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	17	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	17	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	17	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	17	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG21	20	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG22	20	0.19
(1,368)	1:55:A:LEU:HD21	1:78:A:ILE:HG23	20	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG21	20	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG22	20	0.19
(1,368)	1:55:A:LEU:HD22	1:78:A:ILE:HG23	20	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG21	20	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG22	20	0.19
(1,368)	1:55:A:LEU:HD23	1:78:A:ILE:HG23	20	0.19
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	14	0.19
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	6	0.19
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	12	0.19
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	12	0.19
(1,298)	1:24:A:LEU:HD11	1:69:A:ILE:H	3	0.19
(1,298)	1:24:A:LEU:HD12	1:69:A:ILE:H	3	0.19
(1,298)	1:24:A:LEU:HD13	1:69:A:ILE:H	3	0.19
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	16	0.19
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	16	0.19
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	16	0.19
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	16	0.19
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	16	0.19
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	16	0.19
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	3	0.19
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	3	0.19
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	10	0.19
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	10	0.19
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	10	0.19
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	10	0.19
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	10	0.19
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	10	0.19
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	20	0.19
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	20	0.19
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	20	0.19
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG21	2	0.19
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG22	2	0.19
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG23	2	0.19
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG21	2	0.19
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG22	2	0.19
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG23	2	0.19
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG21	2	0.19
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG22	2	0.19
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG23	2	0.19
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	2	0.19
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	2	0.19
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	2	0.19
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD11	4	0.18
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD12	4	0.18
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD13	4	0.18
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	7	0.18
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	13	0.18
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	19	0.18
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	19	0.18
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	13	0.18
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	13	0.18
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	8	0.18
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	1	0.18
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	11	0.18
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE1	18	0.18
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE2	18	0.18
(1,1935)	1:33:A:LEU:HD21	1:33:A:LEU:H	16	0.18
(1,1935)	1:33:A:LEU:HD22	1:33:A:LEU:H	16	0.18
(1,1935)	1:33:A:LEU:HD23	1:33:A:LEU:H	16	0.18
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	3	0.18
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	3	0.18
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	4	0.18
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	4	0.18
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	4	0.18
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB1	19	0.18
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB2	19	0.18
(1,1894)	1:76:A:LYS:H	1:77:A:ALA:HB3	19	0.18
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	10	0.18
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB2	6	0.18
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB3	6	0.18
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB2	12	0.18
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB3	12	0.18
(1,1718)	1:115:A:GLY:H	1:111:A:ASP:HA	5	0.18
(1,1596)	1:102:A:SER:H	1:101:A:HIS:HD2	19	0.18
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	2	0.18
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	4	0.18
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	9	0.18
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	15	0.18
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	3	0.18
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	3	0.18
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	3	0.18
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	8	0.18
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	8	0.18
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	8	0.18
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	15	0.18
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	15	0.18
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	15	0.18
(1,1266)	1:142:A:MET:HE1	1:97:A:GLU:H	9	0.18
(1,1266)	1:142:A:MET:HE2	1:97:A:GLU:H	9	0.18
(1,1266)	1:142:A:MET:HE3	1:97:A:GLU:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	14	0.18
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	14	0.18
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	16	0.18
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	17	0.18
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	7	0.18
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	7	0.18
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	7	0.18
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	7	0.18
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	7	0.18
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	7	0.18
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	2	0.18
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	2	0.18
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	2	0.18
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	2	0.18
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	2	0.18
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	2	0.18
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	2	0.18
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	2	0.18
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	2	0.18
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	9	0.18
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	9	0.18
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	9	0.18
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	9	0.18
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	9	0.18
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	9	0.18
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	6	0.18
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	6	0.18
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	6	0.18
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	12	0.18
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	12	0.18
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	12	0.18
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD2	10	0.18
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD3	10	0.18
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD2	10	0.18
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD3	10	0.18
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD2	10	0.18
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD3	10	0.18
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	6	0.18
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	6	0.18
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	6	0.18
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	6	0.18
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	6	0.18
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	12	0.18
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	12	0.18
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	12	0.18
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	12	0.18
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	12	0.18
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	12	0.18
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	5	0.18
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	5	0.18
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	5	0.18
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	5	0.18
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	5	0.18
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	5	0.18
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	5	0.18
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	5	0.18
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	5	0.18
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	13	0.18
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	13	0.18
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	13	0.18
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	13	0.18
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	13	0.18
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	13	0.18
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	13	0.18
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	13	0.18
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	13	0.18
(1,748)	1:62:A:LEU:HD11	1:45:A:VAL:HA	19	0.18
(1,748)	1:62:A:LEU:HD12	1:45:A:VAL:HA	19	0.18
(1,748)	1:62:A:LEU:HD13	1:45:A:VAL:HA	19	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	1	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	1	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	1	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	1	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	1	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	1	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	1	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	1	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	1	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	17	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	17	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	17	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	17	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	17	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	17	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	17	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	17	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	18	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	18	0.18
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	18	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	18	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	18	0.18
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	18	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	18	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	18	0.18
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	18	0.18
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	15	0.18
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	15	0.18
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	15	0.18
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	18	0.18
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	18	0.18
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	18	0.18
(1,601)	1:39:A:VAL:HG11	1:39:A:VAL:H	18	0.18
(1,601)	1:39:A:VAL:HG12	1:39:A:VAL:H	18	0.18
(1,601)	1:39:A:VAL:HG13	1:39:A:VAL:H	18	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	3	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	3	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	3	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	7	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	7	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	7	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	18	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	18	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	18	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG11	20	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG12	20	0.18
(1,540)	1:27:A:VAL:HA	1:27:A:VAL:HG13	20	0.18
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	9	0.18
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	9	0.18
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	9	0.18
(1,506)	1:23:A:TRP:HD1	1:23:A:TRP:HA	19	0.18
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	13	0.18
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	13	0.18
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	13	0.18
(1,488)	1:15:A:THR:HB	1:16:A:ALA:H	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG21	15	0.18
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG22	15	0.18
(1,479)	1:12:A:VAL:HA	1:12:A:VAL:HG23	15	0.18
(1,409)	1:171:A:GLU:HB2	1:172:A:GLN:H	3	0.18
(1,409)	1:171:A:GLU:HB3	1:172:A:GLN:H	3	0.18
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	1	0.18
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	1	0.18
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	1	0.18
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	11	0.18
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	11	0.18
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	11	0.18
(1,359)	1:42:A:VAL:HB	1:20:A:MET:HA	4	0.18
(1,341)	1:20:A:MET:HE1	1:66:A:ASN:H	4	0.18
(1,341)	1:20:A:MET:HE2	1:66:A:ASN:H	4	0.18
(1,341)	1:20:A:MET:HE3	1:66:A:ASN:H	4	0.18
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	19	0.18
(1,298)	1:24:A:LEU:HD11	1:69:A:ILE:H	2	0.18
(1,298)	1:24:A:LEU:HD12	1:69:A:ILE:H	2	0.18
(1,298)	1:24:A:LEU:HD13	1:69:A:ILE:H	2	0.18
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB2	9	0.18
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB3	9	0.18
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB2	9	0.18
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB3	9	0.18
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB2	9	0.18
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB3	9	0.18
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	1	0.18
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	1	0.18
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	1	0.18
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	4	0.18
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	4	0.18
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	17	0.18
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	17	0.18
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	17	0.18
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD2	4	0.18
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD3	4	0.18
(1,94)	1:58:A:LEU:HA	1:78:A:ILE:HD11	5	0.18
(1,94)	1:58:A:LEU:HA	1:78:A:ILE:HD12	5	0.18
(1,94)	1:58:A:LEU:HA	1:78:A:ILE:HD13	5	0.18
(1,55)	1:45:A:VAL:HA	1:62:A:LEU:H	7	0.18
(1,54)	1:23:A:TRP:H	1:24:A:LEU:H	8	0.18
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG2	9	0.17
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG3	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	13	0.17
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	13	0.17
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	13	0.17
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	8	0.17
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	16	0.17
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	16	0.17
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	4	0.17
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	9	0.17
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	16	0.17
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG21	14	0.17
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG22	14	0.17
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG23	14	0.17
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	5	0.17
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	5	0.17
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD1	9	0.17
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD2	9	0.17
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG21	2	0.17
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG22	2	0.17
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG23	2	0.17
(1,1918)	1:13:A:ARG:H	1:12:A:VAL:HB	15	0.17
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	18	0.17
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	18	0.17
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB2	16	0.17
(1,1832)	1:88:A:ARG:H	1:87:A:ARG:HB3	16	0.17
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB2	4	0.17
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB3	4	0.17
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB2	5	0.17
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB3	5	0.17
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	7	0.17
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	16	0.17
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	16	0.17
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	16	0.17
(1,1681)	1:170:A:ILE:H	1:167:A:ALA:HA	17	0.17
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	8	0.17
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	14	0.17
(1,1547)	1:168:A:ARG:H	1:169:A:PHE:HD1	2	0.17
(1,1547)	1:168:A:ARG:H	1:169:A:PHE:HD2	2	0.17
(1,1520)	1:91:A:GLN:HE22	1:90:A:THR:HB	17	0.17
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG2	2	0.17
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG3	2	0.17
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	13	0.17
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	13	0.17
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	13	0.17
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	13	0.17
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	13	0.17
(1,1279)	1:149:A:ILE:HD11	1:149:A:ILE:HA	1	0.17
(1,1279)	1:149:A:ILE:HD12	1:149:A:ILE:HA	1	0.17
(1,1279)	1:149:A:ILE:HD13	1:149:A:ILE:HA	1	0.17
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	16	0.17
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	16	0.17
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	16	0.17
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	11	0.17
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	11	0.17
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	11	0.17
(1,1159)	1:109:A:ASN:HB2	1:130:A:PRO:HA	3	0.17
(1,1159)	1:109:A:ASN:HB3	1:130:A:PRO:HA	3	0.17
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD21	10	0.17
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD22	10	0.17
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD23	10	0.17
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	18	0.17
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	18	0.17
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	19	0.17
(1,1018)	1:99:A:MET:HG2	1:100:A:ILE:H	20	0.17
(1,1018)	1:99:A:MET:HG3	1:100:A:ILE:H	20	0.17
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	16	0.17
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	16	0.17
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	16	0.17
(1,862)	1:74:A:ASN:HB2	1:138:A:ASN:HD21	11	0.17
(1,862)	1:74:A:ASN:HB3	1:138:A:ASN:HD21	11	0.17
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD11	2	0.17
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD12	2	0.17
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD13	2	0.17
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	3	0.17
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	3	0.17
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	3	0.17
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	3	0.17
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	3	0.17
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	3	0.17
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	3	0.17
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	3	0.17
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	3	0.17
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	18	0.17
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	18	0.17
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	18	0.17
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	18	0.17
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	18	0.17
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	18	0.17
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	18	0.17
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	18	0.17
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	19	0.17
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	3	0.17
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	3	0.17
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	3	0.17
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	3	0.17
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	3	0.17
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	3	0.17
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	3	0.17
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	3	0.17
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	3	0.17
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	20	0.17
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	20	0.17
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	20	0.17
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	20	0.17
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	20	0.17
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	20	0.17
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	20	0.17
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	20	0.17
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	20	0.17
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	6	0.17
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	6	0.17
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	6	0.17
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	12	0.17
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	12	0.17
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	12	0.17
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	13	0.17
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	13	0.17
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	13	0.17
(1,669)	1:47:A:ARG:HD2	1:48:A:ILE:H	11	0.17
(1,669)	1:47:A:ARG:HD3	1:48:A:ILE:H	11	0.17
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	13	0.17
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	13	0.17
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	13	0.17
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	20	0.17
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	20	0.17
(1,637)	1:42:A:VAL:HG21	1:99:A:MET:HA	14	0.17
(1,637)	1:42:A:VAL:HG22	1:99:A:MET:HA	14	0.17
(1,637)	1:42:A:VAL:HG23	1:99:A:MET:HA	14	0.17
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	17	0.17
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	17	0.17
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	17	0.17
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	17	0.17
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	17	0.17
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	17	0.17
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	2	0.17
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	2	0.17
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	2	0.17
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	8	0.17
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	8	0.17
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	8	0.17
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	11	0.17
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	11	0.17
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	11	0.17
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	9	0.17
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	9	0.17
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	9	0.17
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	1	0.17
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	1	0.17
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	1	0.17
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	18	0.17
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	18	0.17
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	18	0.17
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	3	0.17
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	3	0.17
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	3	0.17
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	7	0.17
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	7	0.17
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	7	0.17
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	7	0.17
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	7	0.17
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	17	0.17
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	17	0.17
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	7	0.17
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	7	0.17
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	7	0.17
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	13	0.17
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	13	0.17
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	18	0.17
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	18	0.17
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	18	0.17
(1,364)	1:47:A:ARG:HD2	1:61:A:CYS:H	18	0.17
(1,364)	1:47:A:ARG:HD3	1:61:A:CYS:H	18	0.17
(1,339)	1:8:A:SER:HB2	1:9:A:ARG:HG2	9	0.17
(1,339)	1:8:A:SER:HB2	1:9:A:ARG:HG3	9	0.17
(1,339)	1:8:A:SER:HB3	1:9:A:ARG:HG2	9	0.17
(1,339)	1:8:A:SER:HB3	1:9:A:ARG:HG3	9	0.17
(1,334)	1:26:A:PRO:HB2	1:31:A:ALA:H	13	0.17
(1,334)	1:26:A:PRO:HB3	1:31:A:ALA:H	13	0.17
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	11	0.17
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	7	0.17
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	7	0.17
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	7	0.17
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	19	0.17
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	19	0.17
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	19	0.17
(1,281)	1:42:A:VAL:HB	1:20:A:MET:HG2	7	0.17
(1,281)	1:42:A:VAL:HB	1:20:A:MET:HG3	7	0.17
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE1	6	0.17
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE2	6	0.17
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE1	6	0.17
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE2	6	0.17
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE1	6	0.17
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE2	6	0.17
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE1	12	0.17
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE2	12	0.17
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE1	12	0.17
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE2	12	0.17
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE1	12	0.17
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE2	12	0.17
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	4	0.17
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	4	0.17
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	4	0.17
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	9	0.17
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	9	0.17
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	9	0.17
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	1	0.17
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	8	0.17
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	8	0.17
(1,179)	1:24:A:LEU:HG	1:25:A:GLU:H	17	0.17
(1,161)	1:156:A:ILE:HG21	1:63:A:CYS:HB2	1	0.17
(1,161)	1:156:A:ILE:HG21	1:63:A:CYS:HB3	1	0.17
(1,161)	1:156:A:ILE:HG22	1:63:A:CYS:HB2	1	0.17
(1,161)	1:156:A:ILE:HG22	1:63:A:CYS:HB3	1	0.17
(1,161)	1:156:A:ILE:HG23	1:63:A:CYS:HB2	1	0.17
(1,161)	1:156:A:ILE:HG23	1:63:A:CYS:HB3	1	0.17
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB1	14	0.17
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB2	14	0.17
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB3	14	0.17
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB1	14	0.17
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB2	14	0.17
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB3	14	0.17
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB1	14	0.17
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB2	14	0.17
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB3	14	0.17
(1,48)	1:150:A:LEU:HD11	1:46:A:LEU:HD11	16	0.17
(1,48)	1:150:A:LEU:HD11	1:46:A:LEU:HD12	16	0.17
(1,48)	1:150:A:LEU:HD11	1:46:A:LEU:HD13	16	0.17
(1,48)	1:150:A:LEU:HD12	1:46:A:LEU:HD11	16	0.17
(1,48)	1:150:A:LEU:HD12	1:46:A:LEU:HD12	16	0.17
(1,48)	1:150:A:LEU:HD12	1:46:A:LEU:HD13	16	0.17
(1,48)	1:150:A:LEU:HD13	1:46:A:LEU:HD11	16	0.17
(1,48)	1:150:A:LEU:HD13	1:46:A:LEU:HD12	16	0.17
(1,48)	1:150:A:LEU:HD13	1:46:A:LEU:HD13	16	0.17
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG21	13	0.17
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG22	13	0.17
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG23	13	0.17
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG21	13	0.17
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG22	13	0.17
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG23	13	0.17
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG21	13	0.17
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG22	13	0.17
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG23	13	0.17
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	13	0.17
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	13	0.17
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	13	0.17
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	13	0.17
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	13	0.17
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:105:A:ILE:HG12	1:169:A:PHE:HE1	3	0.17
(1,28)	1:105:A:ILE:HG12	1:169:A:PHE:HE2	3	0.17
(1,28)	1:105:A:ILE:HG13	1:169:A:PHE:HE1	3	0.17
(1,28)	1:105:A:ILE:HG13	1:169:A:PHE:HE2	3	0.17
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD11	17	0.17
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD12	17	0.17
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD13	17	0.17
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD11	17	0.17
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD12	17	0.17
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD13	17	0.17
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD11	17	0.17
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD12	17	0.17
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD13	17	0.17
(1,13)	1:142:A:MET:HE1	1:94:A:LEU:HG	11	0.17
(1,13)	1:142:A:MET:HE2	1:94:A:LEU:HG	11	0.17
(1,13)	1:142:A:MET:HE3	1:94:A:LEU:HG	11	0.17
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD11	1	0.16
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD12	1	0.16
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD13	1	0.16
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	4	0.16
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	4	0.16
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	4	0.16
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	15	0.16
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	15	0.16
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	15	0.16
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	3	0.16
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	10	0.16
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB2	19	0.16
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB3	19	0.16
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	2	0.16
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	18	0.16
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	4	0.16
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	4	0.16
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	19	0.16
(1,1881)	1:174:A:PHE:HB2	1:174:A:PHE:H	19	0.16
(1,1881)	1:174:A:PHE:HB3	1:174:A:PHE:H	19	0.16
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB2	13	0.16
(1,1875)	1:177:A:GLU:H	1:176:A:ASP:HB3	13	0.16
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	14	0.16
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	14	0.16
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	14	0.16
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	20	0.16
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	20	0.16
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	11	0.16
(1,1758)	1:54:A:THR:HG21	1:55:A:LEU:H	1	0.16
(1,1758)	1:54:A:THR:HG22	1:55:A:LEU:H	1	0.16
(1,1758)	1:54:A:THR:HG23	1:55:A:LEU:H	1	0.16
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	5	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	6	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	6	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	6	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	12	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	12	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	12	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	16	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	16	0.16
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	16	0.16
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	7	0.16
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	18	0.16
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	20	0.16
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	3	0.16
(1,1423)	1:170:A:ILE:HG21	1:171:A:GLU:HA	20	0.16
(1,1423)	1:170:A:ILE:HG22	1:171:A:GLU:HA	20	0.16
(1,1423)	1:170:A:ILE:HG23	1:171:A:GLU:HA	20	0.16
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	4	0.16
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	4	0.16
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	4	0.16
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	4	0.16
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	4	0.16
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	4	0.16
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	17	0.16
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	17	0.16
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	17	0.16
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	17	0.16
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	17	0.16
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	17	0.16
(1,1306)	1:155:A:THR:HG21	1:156:A:ILE:HB	20	0.16
(1,1306)	1:155:A:THR:HG22	1:156:A:ILE:HB	20	0.16
(1,1306)	1:155:A:THR:HG23	1:156:A:ILE:HB	20	0.16
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	5	0.16
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	13	0.16
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	13	0.16
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	1	0.16
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	1	0.16
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	1	0.16
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	1	0.16
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	1	0.16
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	1	0.16
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	6	0.16
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	6	0.16
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	6	0.16
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	7	0.16
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	7	0.16
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	7	0.16
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	12	0.16
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	12	0.16
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	12	0.16
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	10	0.16
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	10	0.16
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	10	0.16
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	3	0.16
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	3	0.16
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	8	0.16
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	19	0.16
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	19	0.16
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	19	0.16
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	19	0.16
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	19	0.16
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	19	0.16
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	19	0.16
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	19	0.16
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	19	0.16
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD1	10	0.16
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD2	10	0.16
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD1	10	0.16
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD2	10	0.16
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD1	10	0.16
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD2	10	0.16
(1,1012)	1:99:A:MET:HE1	1:99:A:MET:HA	20	0.16
(1,1012)	1:99:A:MET:HE2	1:99:A:MET:HA	20	0.16
(1,1012)	1:99:A:MET:HE3	1:99:A:MET:HA	20	0.16
(1,974)	1:45:A:VAL:HG21	1:95:A:ASN:H	3	0.16
(1,974)	1:45:A:VAL:HG22	1:95:A:ASN:H	3	0.16
(1,974)	1:45:A:VAL:HG23	1:95:A:ASN:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	3	0.16
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	3	0.16
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	3	0.16
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	9	0.16
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	9	0.16
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	9	0.16
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	13	0.16
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	13	0.16
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	13	0.16
(1,951)	1:89:A:VAL:HG21	1:140:A:PHE:HZ	4	0.16
(1,951)	1:89:A:VAL:HG22	1:140:A:PHE:HZ	4	0.16
(1,951)	1:89:A:VAL:HG23	1:140:A:PHE:HZ	4	0.16
(1,862)	1:74:A:ASN:HB2	1:138:A:ASN:HD21	6	0.16
(1,862)	1:74:A:ASN:HB3	1:138:A:ASN:HD21	6	0.16
(1,862)	1:74:A:ASN:HB2	1:138:A:ASN:HD21	12	0.16
(1,862)	1:74:A:ASN:HB3	1:138:A:ASN:HD21	12	0.16
(1,854)	1:73:A:ALA:HB1	1:140:A:PHE:HZ	4	0.16
(1,854)	1:73:A:ALA:HB2	1:140:A:PHE:HZ	4	0.16
(1,854)	1:73:A:ALA:HB3	1:140:A:PHE:HZ	4	0.16
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	3	0.16
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	3	0.16
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	3	0.16
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	3	0.16
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	3	0.16
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	3	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	6	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	6	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	6	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	6	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	6	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	6	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	6	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	6	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	6	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	12	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	12	0.16
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	12	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	12	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	12	0.16
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	12	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	12	0.16
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	12	0.16
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD21	1	0.16
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD22	1	0.16
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD23	1	0.16
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD21	1	0.16
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD22	1	0.16
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD23	1	0.16
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD21	1	0.16
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD22	1	0.16
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD23	1	0.16
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	7	0.16
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	7	0.16
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	7	0.16
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	7	0.16
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	7	0.16
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	7	0.16
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	7	0.16
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	7	0.16
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	7	0.16
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	8	0.16
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	8	0.16
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	8	0.16
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	8	0.16
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	8	0.16
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	8	0.16
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	8	0.16
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	8	0.16
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	8	0.16
(1,700)	1:55:A:LEU:HD11	1:55:A:LEU:H	5	0.16
(1,700)	1:55:A:LEU:HD12	1:55:A:LEU:H	5	0.16
(1,700)	1:55:A:LEU:HD13	1:55:A:LEU:H	5	0.16
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	7	0.16
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	7	0.16
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	7	0.16
(1,660)	1:46:A:LEU:HD21	1:46:A:LEU:HA	5	0.16
(1,660)	1:46:A:LEU:HD22	1:46:A:LEU:HA	5	0.16
(1,660)	1:46:A:LEU:HD23	1:46:A:LEU:HA	5	0.16
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	3	0.16
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	3	0.16
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	3	0.16
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	6	0.16
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	6	0.16
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	12	0.16
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	12	0.16
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	12	0.16
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	19	0.16
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	19	0.16
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	19	0.16
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	11	0.16
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	11	0.16
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	11	0.16
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG12	20	0.16
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG13	20	0.16
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG12	20	0.16
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG13	20	0.16
(1,425)	1:62:A:LEU:HD11	1:43:A:LEU:HA	18	0.16
(1,425)	1:62:A:LEU:HD12	1:43:A:LEU:HA	18	0.16
(1,425)	1:62:A:LEU:HD13	1:43:A:LEU:HA	18	0.16
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	3	0.16
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	3	0.16
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	3	0.16
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	4	0.16
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	4	0.16
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	4	0.16
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	5	0.16
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	5	0.16
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	5	0.16
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB1	5	0.16
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB2	5	0.16
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB3	5	0.16
(1,298)	1:24:A:LEU:HD11	1:69:A:ILE:H	9	0.16
(1,298)	1:24:A:LEU:HD12	1:69:A:ILE:H	9	0.16
(1,298)	1:24:A:LEU:HD13	1:69:A:ILE:H	9	0.16
(1,298)	1:24:A:LEU:HD11	1:69:A:ILE:H	11	0.16
(1,298)	1:24:A:LEU:HD12	1:69:A:ILE:H	11	0.16
(1,298)	1:24:A:LEU:HD13	1:69:A:ILE:H	11	0.16
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	1	0.16
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	1	0.16
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	1	0.16
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	11	0.16
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	11	0.16
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	11	0.16
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	13	0.16
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	13	0.16
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	10	0.16
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	10	0.16
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	10	0.16
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD1	13	0.16
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD2	13	0.16
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD1	13	0.16
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD2	13	0.16
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE1	14	0.16
(1,244)	1:78:A:ILE:HG21	1:75:A:TYR:HE2	14	0.16
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE1	14	0.16
(1,244)	1:78:A:ILE:HG22	1:75:A:TYR:HE2	14	0.16
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE1	14	0.16
(1,244)	1:78:A:ILE:HG23	1:75:A:TYR:HE2	14	0.16
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	11	0.16
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	11	0.16
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	11	0.16
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	16	0.16
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	16	0.16
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD1	7	0.16
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD2	7	0.16
(1,183)	1:135:A:LEU:HD21	1:23:A:TRP:HH2	8	0.16
(1,183)	1:135:A:LEU:HD22	1:23:A:TRP:HH2	8	0.16
(1,183)	1:135:A:LEU:HD23	1:23:A:TRP:HH2	8	0.16
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	7	0.16
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	7	0.16
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	7	0.16
(1,115)	1:119:A:GLY:HA2	1:114:A:GLN:HG2	5	0.16
(1,115)	1:119:A:GLY:HA2	1:114:A:GLN:HG3	5	0.16
(1,115)	1:119:A:GLY:HA3	1:114:A:GLN:HG2	5	0.16
(1,115)	1:119:A:GLY:HA3	1:114:A:GLN:HG3	5	0.16
(1,95)	1:8:A:SER:HA	1:11:A:ALA:HB1	2	0.16
(1,95)	1:8:A:SER:HA	1:11:A:ALA:HB2	2	0.16
(1,95)	1:8:A:SER:HA	1:11:A:ALA:HB3	2	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD11	6	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD12	6	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD13	6	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD11	12	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD12	12	0.16
(1,60)	1:120:A:LEU:HA	1:120:A:LEU:HD13	12	0.16
(1,40)	1:33:A:LEU:HD21	1:39:A:VAL:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:33:A:LEU:HD22	1:39:A:VAL:H	7	0.16
(1,40)	1:33:A:LEU:HD23	1:39:A:VAL:H	7	0.16
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	9	0.16
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	9	0.16
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	9	0.16
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	4	0.16
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	4	0.16
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	4	0.16
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	4	0.16
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	4	0.16
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	4	0.16
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	11	0.16
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	11	0.16
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	11	0.16
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	11	0.16
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	11	0.16
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	11	0.16
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD11	14	0.15
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD12	14	0.15
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD13	14	0.15
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD11	19	0.15
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD12	19	0.15
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD13	19	0.15
(1,2180)	1:140:A:PHE:HD1	1:142:A:MET:H	13	0.15
(1,2180)	1:140:A:PHE:HD2	1:142:A:MET:H	13	0.15
(1,2179)	1:142:A:MET:H	1:84:A:LYS:HB2	16	0.15
(1,2179)	1:142:A:MET:H	1:84:A:LYS:HB3	16	0.15
(1,2125)	1:103:A:PHE:H	1:38:A:LYS:HG2	18	0.15
(1,2125)	1:103:A:PHE:H	1:38:A:LYS:HG3	18	0.15
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	11	0.15
(1,2114)	1:72:A:PHE:HD1	1:72:A:PHE:H	20	0.15
(1,2114)	1:72:A:PHE:HD2	1:72:A:PHE:H	20	0.15
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	1	0.15
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	14	0.15
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE1	13	0.15
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE2	13	0.15
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	15	0.15
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	15	0.15
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG11	15	0.15
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG12	15	0.15
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG13	15	0.15
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG21	9	0.15
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG22	9	0.15
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG23	9	0.15
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	2	0.15
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	2	0.15
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	4	0.15
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	4	0.15
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB2	8	0.15
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB3	8	0.15
(1,1726)	1:166:A:ILE:HA	1:171:A:GLU:H	13	0.15
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	2	0.15
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	20	0.15
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB2	17	0.15
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB3	17	0.15
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	2	0.15
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	18	0.15
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	18	0.15
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	18	0.15
(1,1633)	1:156:A:ILE:HB	1:155:A:THR:H	17	0.15
(1,1621)	1:91:A:GLN:HE21	1:88:A:ARG:HA	17	0.15
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	3	0.15
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	16	0.15
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	18	0.15
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD11	11	0.15
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD12	11	0.15
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD13	11	0.15
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG21	14	0.15
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG22	14	0.15
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG23	14	0.15
(1,1411)	1:170:A:ILE:HD11	1:129:A:PHE:HD1	16	0.15
(1,1411)	1:170:A:ILE:HD11	1:129:A:PHE:HD2	16	0.15
(1,1411)	1:170:A:ILE:HD12	1:129:A:PHE:HD1	16	0.15
(1,1411)	1:170:A:ILE:HD12	1:129:A:PHE:HD2	16	0.15
(1,1411)	1:170:A:ILE:HD13	1:129:A:PHE:HD1	16	0.15
(1,1411)	1:170:A:ILE:HD13	1:129:A:PHE:HD2	16	0.15
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	5	0.15
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	5	0.15
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	5	0.15
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	6	0.15
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	6	0.15
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	6	0.15
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	12	0.15
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	12	0.15
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	13	0.15
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	13	0.15
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	13	0.15
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	9	0.15
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	9	0.15
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	9	0.15
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	19	0.15
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	19	0.15
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	19	0.15
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	17	0.15
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	17	0.15
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	17	0.15
(1,1159)	1:109:A:ASN:HB2	1:130:A:PRO:HA	4	0.15
(1,1159)	1:109:A:ASN:HB3	1:130:A:PRO:HA	4	0.15
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	4	0.15
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	10	0.15
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	18	0.15
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	4	0.15
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	4	0.15
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	4	0.15
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	4	0.15
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	4	0.15
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	4	0.15
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	14	0.15
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	14	0.15
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	14	0.15
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	14	0.15
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	14	0.15
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	14	0.15
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	14	0.15
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	14	0.15
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	14	0.15
(1,1018)	1:99:A:MET:HG2	1:100:A:ILE:H	17	0.15
(1,1018)	1:99:A:MET:HG3	1:100:A:ILE:H	17	0.15
(1,1016)	1:99:A:MET:HE1	1:143:A:PHE:HZ	11	0.15
(1,1016)	1:99:A:MET:HE2	1:143:A:PHE:HZ	11	0.15
(1,1016)	1:99:A:MET:HE3	1:143:A:PHE:HZ	11	0.15
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	3	0.15
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	3	0.15
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	3	0.15
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	3	0.15
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	3	0.15
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	4	0.15
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	4	0.15
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	4	0.15
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	4	0.15
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	4	0.15
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	4	0.15
(1,1005)	1:98:A:ILE:HG21	1:143:A:PHE:H	4	0.15
(1,1005)	1:98:A:ILE:HG22	1:143:A:PHE:H	4	0.15
(1,1005)	1:98:A:ILE:HG23	1:143:A:PHE:H	4	0.15
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	10	0.15
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	10	0.15
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	10	0.15
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	11	0.15
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	11	0.15
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	11	0.15
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	16	0.15
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	16	0.15
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	16	0.15
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD2	11	0.15
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD3	11	0.15
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD2	11	0.15
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD3	11	0.15
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD2	11	0.15
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD3	11	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	3	0.15
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	3	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	5	0.15
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	5	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	6	0.15
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	6	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	8	0.15
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	8	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	12	0.15
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	12	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	15	0.15
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	15	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	16	0.15
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	16	0.15
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	17	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	10	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	10	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	10	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	10	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	10	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	10	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	10	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	10	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	10	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	11	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	11	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	11	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	11	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	11	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	11	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	11	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	11	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	11	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	19	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	19	0.15
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	19	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	19	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	19	0.15
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	19	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	19	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	19	0.15
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	19	0.15
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	3	0.15
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	4	0.15
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	13	0.15
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	20	0.15
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG2	11	0.15
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG3	11	0.15
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	5	0.15
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	5	0.15
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	5	0.15
(1,655)	1:42:A:VAL:HG21	1:100:A:ILE:H	4	0.15
(1,655)	1:42:A:VAL:HG22	1:100:A:ILE:H	4	0.15
(1,655)	1:42:A:VAL:HG23	1:100:A:ILE:H	4	0.15
(1,631)	1:42:A:VAL:HG11	1:143:A:PHE:HD1	20	0.15
(1,631)	1:42:A:VAL:HG11	1:143:A:PHE:HD2	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:42:A:VAL:HG12	1:143:A:PHE:HD1	20	0.15
(1,631)	1:42:A:VAL:HG12	1:143:A:PHE:HD2	20	0.15
(1,631)	1:42:A:VAL:HG13	1:143:A:PHE:HD1	20	0.15
(1,631)	1:42:A:VAL:HG13	1:143:A:PHE:HD2	20	0.15
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	7	0.15
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	7	0.15
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	7	0.15
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	7	0.15
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	7	0.15
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	7	0.15
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	16	0.15
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	16	0.15
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	16	0.15
(1,573)	1:33:A:LEU:HD11	1:33:A:LEU:H	5	0.15
(1,573)	1:33:A:LEU:HD12	1:33:A:LEU:H	5	0.15
(1,573)	1:33:A:LEU:HD13	1:33:A:LEU:H	5	0.15
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	10	0.15
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	10	0.15
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	10	0.15
(1,497)	1:20:A:MET:HE1	1:42:A:VAL:HG11	4	0.15
(1,497)	1:20:A:MET:HE1	1:42:A:VAL:HG12	4	0.15
(1,497)	1:20:A:MET:HE1	1:42:A:VAL:HG13	4	0.15
(1,497)	1:20:A:MET:HE2	1:42:A:VAL:HG11	4	0.15
(1,497)	1:20:A:MET:HE2	1:42:A:VAL:HG12	4	0.15
(1,497)	1:20:A:MET:HE2	1:42:A:VAL:HG13	4	0.15
(1,497)	1:20:A:MET:HE3	1:42:A:VAL:HG11	4	0.15
(1,497)	1:20:A:MET:HE3	1:42:A:VAL:HG12	4	0.15
(1,497)	1:20:A:MET:HE3	1:42:A:VAL:HG13	4	0.15
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD1	18	0.15
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD2	18	0.15
(1,455)	1:20:A:MET:HE1	1:43:A:LEU:HD11	10	0.15
(1,455)	1:20:A:MET:HE1	1:43:A:LEU:HD12	10	0.15
(1,455)	1:20:A:MET:HE1	1:43:A:LEU:HD13	10	0.15
(1,455)	1:20:A:MET:HE2	1:43:A:LEU:HD11	10	0.15
(1,455)	1:20:A:MET:HE2	1:43:A:LEU:HD12	10	0.15
(1,455)	1:20:A:MET:HE2	1:43:A:LEU:HD13	10	0.15
(1,455)	1:20:A:MET:HE3	1:43:A:LEU:HD11	10	0.15
(1,455)	1:20:A:MET:HE3	1:43:A:LEU:HD12	10	0.15
(1,455)	1:20:A:MET:HE3	1:43:A:LEU:HD13	10	0.15
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	10	0.15
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	10	0.15
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:62:A:LEU:HD11	1:43:A:LEU:HA	3	0.15
(1,425)	1:62:A:LEU:HD12	1:43:A:LEU:HA	3	0.15
(1,425)	1:62:A:LEU:HD13	1:43:A:LEU:HA	3	0.15
(1,418)	1:72:A:PHE:HB2	1:60:A:LEU:H	4	0.15
(1,418)	1:72:A:PHE:HB3	1:60:A:LEU:H	4	0.15
(1,409)	1:171:A:GLU:HB2	1:172:A:GLN:H	17	0.15
(1,409)	1:171:A:GLU:HB3	1:172:A:GLN:H	17	0.15
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	16	0.15
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	16	0.15
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD1	20	0.15
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD2	20	0.15
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD1	20	0.15
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD2	20	0.15
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	3	0.15
(1,302)	1:15:A:THR:HG21	1:15:A:THR:HA	16	0.15
(1,302)	1:15:A:THR:HG22	1:15:A:THR:HA	16	0.15
(1,302)	1:15:A:THR:HG23	1:15:A:THR:HA	16	0.15
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG21	14	0.15
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG22	14	0.15
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG23	14	0.15
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG21	14	0.15
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG22	14	0.15
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG23	14	0.15
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG21	14	0.15
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG22	14	0.15
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG23	14	0.15
(1,298)	1:24:A:LEU:HD11	1:69:A:ILE:H	17	0.15
(1,298)	1:24:A:LEU:HD12	1:69:A:ILE:H	17	0.15
(1,298)	1:24:A:LEU:HD13	1:69:A:ILE:H	17	0.15
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	6	0.15
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	6	0.15
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	6	0.15
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	12	0.15
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	12	0.15
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	12	0.15
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB2	10	0.15
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB3	10	0.15
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB2	10	0.15
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB3	10	0.15
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB2	10	0.15
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB3	10	0.15
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	8	0.15
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	8	0.15
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	13	0.15
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	13	0.15
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	13	0.15
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	10	0.15
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	10	0.15
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	10	0.15
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	19	0.15
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	19	0.15
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	19	0.15
(1,251)	1:76:A:LYS:HG2	1:74:A:ASN:HD21	17	0.15
(1,251)	1:76:A:LYS:HG2	1:74:A:ASN:HD22	17	0.15
(1,251)	1:76:A:LYS:HG3	1:74:A:ASN:HD21	17	0.15
(1,251)	1:76:A:LYS:HG3	1:74:A:ASN:HD22	17	0.15
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	10	0.15
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	10	0.15
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	10	0.15
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	10	0.15
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	10	0.15
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	10	0.15
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	20	0.15
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	20	0.15
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	7	0.15
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	7	0.15
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	7	0.15
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD21	1	0.15
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD22	1	0.15
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD23	1	0.15
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD21	1	0.15
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD22	1	0.15
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD23	1	0.15
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD21	1	0.15
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD22	1	0.15
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD23	1	0.15
(1,183)	1:135:A:LEU:HD21	1:23:A:TRP:HH2	5	0.15
(1,183)	1:135:A:LEU:HD22	1:23:A:TRP:HH2	5	0.15
(1,183)	1:135:A:LEU:HD23	1:23:A:TRP:HH2	5	0.15
(1,183)	1:135:A:LEU:HD21	1:23:A:TRP:HH2	9	0.15
(1,183)	1:135:A:LEU:HD22	1:23:A:TRP:HH2	9	0.15
(1,183)	1:135:A:LEU:HD23	1:23:A:TRP:HH2	9	0.15
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD1	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD2	4	0.15
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD1	4	0.15
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD2	4	0.15
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD1	4	0.15
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD2	4	0.15
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	1	0.15
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	1	0.15
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	1	0.15
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	1	0.15
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	1	0.15
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	1	0.15
(1,150)	1:166:A:ILE:HG21	1:170:A:ILE:H	15	0.15
(1,150)	1:166:A:ILE:HG22	1:170:A:ILE:H	15	0.15
(1,150)	1:166:A:ILE:HG23	1:170:A:ILE:H	15	0.15
(1,148)	1:167:A:ALA:HB1	1:164:A:ARG:HD2	4	0.15
(1,148)	1:167:A:ALA:HB1	1:164:A:ARG:HD3	4	0.15
(1,148)	1:167:A:ALA:HB2	1:164:A:ARG:HD2	4	0.15
(1,148)	1:167:A:ALA:HB2	1:164:A:ARG:HD3	4	0.15
(1,148)	1:167:A:ALA:HB3	1:164:A:ARG:HD2	4	0.15
(1,148)	1:167:A:ALA:HB3	1:164:A:ARG:HD3	4	0.15
(1,148)	1:167:A:ALA:HB1	1:164:A:ARG:HD2	20	0.15
(1,148)	1:167:A:ALA:HB1	1:164:A:ARG:HD3	20	0.15
(1,148)	1:167:A:ALA:HB2	1:164:A:ARG:HD2	20	0.15
(1,148)	1:167:A:ALA:HB2	1:164:A:ARG:HD3	20	0.15
(1,148)	1:167:A:ALA:HB3	1:164:A:ARG:HD2	20	0.15
(1,148)	1:167:A:ALA:HB3	1:164:A:ARG:HD3	20	0.15
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	1	0.15
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	1	0.15
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	1	0.15
(1,122)	1:114:A:GLN:HA	1:119:A:GLY:H	15	0.15
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	6	0.15
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	6	0.15
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	6	0.15
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	10	0.15
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	10	0.15
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	10	0.15
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	12	0.15
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	12	0.15
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	12	0.15
(1,40)	1:33:A:LEU:HD21	1:39:A:VAL:H	5	0.15
(1,40)	1:33:A:LEU:HD22	1:39:A:VAL:H	5	0.15
(1,40)	1:33:A:LEU:HD23	1:39:A:VAL:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:33:A:LEU:HD21	1:39:A:VAL:H	13	0.15
(1,40)	1:33:A:LEU:HD22	1:39:A:VAL:H	13	0.15
(1,40)	1:33:A:LEU:HD23	1:39:A:VAL:H	13	0.15
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD1	9	0.15
(1,37)	1:33:A:LEU:HD11	1:37:A:TYR:HD2	9	0.15
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD1	9	0.15
(1,37)	1:33:A:LEU:HD12	1:37:A:TYR:HD2	9	0.15
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD1	9	0.15
(1,37)	1:33:A:LEU:HD13	1:37:A:TYR:HD2	9	0.15
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	16	0.15
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	16	0.15
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	16	0.15
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	16	0.15
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	16	0.15
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	16	0.15
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	5	0.15
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	5	0.15
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	5	0.15
(1,27)	1:167:A:ALA:HA	1:171:A:GLU:H	15	0.15
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD11	9	0.15
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD12	9	0.15
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD13	9	0.15
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD11	9	0.15
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD12	9	0.15
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD13	9	0.15
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD11	9	0.15
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD12	9	0.15
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD13	9	0.15
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD2	15	0.14
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD3	15	0.14
(1,2258)	1:137:A:ILE:HA	1:104:A:THR:H	17	0.14
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD11	20	0.14
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD12	20	0.14
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD13	20	0.14
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	4	0.14
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	4	0.14
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	4	0.14
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB1	6	0.14
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB2	6	0.14
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB3	6	0.14
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB1	12	0.14
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB2	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB3	12	0.14
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	20	0.14
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	8	0.14
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	8	0.14
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	8	0.14
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD11	19	0.14
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD12	19	0.14
(1,2168)	1:63:A:CYS:H	1:46:A:LEU:HD13	19	0.14
(1,2153)	1:136:A:GLU:H	1:105:A:ILE:HA	7	0.14
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	17	0.14
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	19	0.14
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	6	0.14
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	10	0.14
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	12	0.14
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	13	0.14
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	17	0.14
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	19	0.14
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	5	0.14
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	9	0.14
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	20	0.14
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	10	0.14
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	10	0.14
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG11	14	0.14
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG12	14	0.14
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG13	14	0.14
(1,1999)	1:149:A:ILE:HD11	1:149:A:ILE:H	10	0.14
(1,1999)	1:149:A:ILE:HD12	1:149:A:ILE:H	10	0.14
(1,1999)	1:149:A:ILE:HD13	1:149:A:ILE:H	10	0.14
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD1	20	0.14
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD2	20	0.14
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	17	0.14
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	17	0.14
(1,1854)	1:146:A:ASP:H	1:147:A:GLN:H	1	0.14
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD1	2	0.14
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD2	2	0.14
(1,1801)	1:41:A:LYS:HD2	1:42:A:VAL:H	10	0.14
(1,1801)	1:41:A:LYS:HD3	1:42:A:VAL:H	10	0.14
(1,1793)	1:91:A:GLN:H	1:89:A:VAL:HG11	16	0.14
(1,1793)	1:91:A:GLN:H	1:89:A:VAL:HG12	16	0.14
(1,1793)	1:91:A:GLN:H	1:89:A:VAL:HG13	16	0.14
(1,1786)	1:124:A:GLN:HG2	1:125:A:LYS:H	18	0.14
(1,1786)	1:124:A:GLN:HG3	1:125:A:LYS:H	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB2	10	0.14
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB3	10	0.14
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB2	17	0.14
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB3	17	0.14
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	8	0.14
(1,1759)	1:54:A:THR:HB	1:55:A:LEU:H	3	0.14
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	4	0.14
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB2	2	0.14
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB3	2	0.14
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB2	15	0.14
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB3	15	0.14
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	13	0.14
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	13	0.14
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	17	0.14
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	17	0.14
(1,1681)	1:170:A:ILE:H	1:167:A:ALA:HA	5	0.14
(1,1681)	1:170:A:ILE:H	1:167:A:ALA:HA	15	0.14
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	13	0.14
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	17	0.14
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	19	0.14
(1,1569)	1:82:A:GLU:HA	1:87:A:ARG:H	9	0.14
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	4	0.14
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD11	7	0.14
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD12	7	0.14
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD13	7	0.14
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG21	4	0.14
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG22	4	0.14
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG23	4	0.14
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD11	15	0.14
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD12	15	0.14
(1,1451)	1:160:A:TYR:H	1:159:A:LEU:HD13	15	0.14
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG2	7	0.14
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG3	7	0.14
(1,1425)	1:171:A:GLU:HA	1:174:A:PHE:HB2	9	0.14
(1,1425)	1:171:A:GLU:HA	1:174:A:PHE:HB3	9	0.14
(1,1423)	1:170:A:ILE:HG21	1:171:A:GLU:HA	3	0.14
(1,1423)	1:170:A:ILE:HG22	1:171:A:GLU:HA	3	0.14
(1,1423)	1:170:A:ILE:HG23	1:171:A:GLU:HA	3	0.14
(1,1423)	1:170:A:ILE:HG21	1:171:A:GLU:HA	6	0.14
(1,1423)	1:170:A:ILE:HG22	1:171:A:GLU:HA	6	0.14
(1,1423)	1:170:A:ILE:HG23	1:171:A:GLU:HA	6	0.14
(1,1423)	1:170:A:ILE:HG21	1:171:A:GLU:HA	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:170:A:ILE:HG22	1:171:A:GLU:HA	12	0.14
(1,1423)	1:170:A:ILE:HG23	1:171:A:GLU:HA	12	0.14
(1,1423)	1:170:A:ILE:HG21	1:171:A:GLU:HA	19	0.14
(1,1423)	1:170:A:ILE:HG22	1:171:A:GLU:HA	19	0.14
(1,1423)	1:170:A:ILE:HG23	1:171:A:GLU:HA	19	0.14
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	15	0.14
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	15	0.14
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	15	0.14
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	15	0.14
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	15	0.14
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	15	0.14
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	16	0.14
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	16	0.14
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	16	0.14
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	16	0.14
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	16	0.14
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	16	0.14
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	19	0.14
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG21	5	0.14
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG22	5	0.14
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG23	5	0.14
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG21	5	0.14
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG22	5	0.14
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG23	5	0.14
(1,1248)	1:140:A:PHE:HA	1:102:A:SER:H	8	0.14
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	9	0.14
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	9	0.14
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	9	0.14
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	17	0.14
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	17	0.14
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	17	0.14
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	20	0.14
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	20	0.14
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	20	0.14
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	5	0.14
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	5	0.14
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	5	0.14
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	14	0.14
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	14	0.14
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	14	0.14
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	19	0.14
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	19	0.14
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	3	0.14
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	3	0.14
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	3	0.14
(1,1167)	1:131:A:GLY:HA2	1:129:A:PHE:HE1	5	0.14
(1,1167)	1:131:A:GLY:HA2	1:129:A:PHE:HE2	5	0.14
(1,1167)	1:131:A:GLY:HA3	1:129:A:PHE:HE1	5	0.14
(1,1167)	1:131:A:GLY:HA3	1:129:A:PHE:HE2	5	0.14
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	2	0.14
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	2	0.14
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	5	0.14
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	6	0.14
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	12	0.14
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	20	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	3	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	3	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	3	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	3	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	3	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	3	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	10	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	10	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	10	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	10	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	10	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	10	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	17	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	17	0.14
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	17	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	17	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	17	0.14
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	17	0.14
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	15	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	13	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	13	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	13	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	14	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	14	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	14	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	16	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	16	0.14
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	10	0.14
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	10	0.14
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	10	0.14
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	10	0.14
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	10	0.14
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	10	0.14
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD1	18	0.14
(1,1014)	1:99:A:MET:HE1	1:143:A:PHE:HD2	18	0.14
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD1	18	0.14
(1,1014)	1:99:A:MET:HE2	1:143:A:PHE:HD2	18	0.14
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD1	18	0.14
(1,1014)	1:99:A:MET:HE3	1:143:A:PHE:HD2	18	0.14
(1,1012)	1:99:A:MET:HE1	1:99:A:MET:HA	11	0.14
(1,1012)	1:99:A:MET:HE2	1:99:A:MET:HA	11	0.14
(1,1012)	1:99:A:MET:HE3	1:99:A:MET:HA	11	0.14
(1,990)	1:45:A:VAL:HG11	1:98:A:ILE:HD11	17	0.14
(1,990)	1:45:A:VAL:HG11	1:98:A:ILE:HD12	17	0.14
(1,990)	1:45:A:VAL:HG11	1:98:A:ILE:HD13	17	0.14
(1,990)	1:45:A:VAL:HG12	1:98:A:ILE:HD11	17	0.14
(1,990)	1:45:A:VAL:HG12	1:98:A:ILE:HD12	17	0.14
(1,990)	1:45:A:VAL:HG12	1:98:A:ILE:HD13	17	0.14
(1,990)	1:45:A:VAL:HG13	1:98:A:ILE:HD11	17	0.14
(1,990)	1:45:A:VAL:HG13	1:98:A:ILE:HD12	17	0.14
(1,990)	1:45:A:VAL:HG13	1:98:A:ILE:HD13	17	0.14
(1,956)	1:90:A:THR:HB	1:58:A:LEU:HD21	18	0.14
(1,956)	1:90:A:THR:HB	1:58:A:LEU:HD22	18	0.14
(1,956)	1:90:A:THR:HB	1:58:A:LEU:HD23	18	0.14
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	8	0.14
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	8	0.14
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	8	0.14
(1,951)	1:89:A:VAL:HG21	1:140:A:PHE:HZ	9	0.14
(1,951)	1:89:A:VAL:HG22	1:140:A:PHE:HZ	9	0.14
(1,951)	1:89:A:VAL:HG23	1:140:A:PHE:HZ	9	0.14
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	4	0.14
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	4	0.14
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	7	0.14
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	7	0.14
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	9	0.14
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	9	0.14
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	10	0.14
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	10	0.14
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	14	0.14
(1,849)	1:73:A:ALA:HB1	1:74:A:ASN:H	13	0.14
(1,849)	1:73:A:ALA:HB2	1:74:A:ASN:H	13	0.14
(1,849)	1:73:A:ALA:HB3	1:74:A:ASN:H	13	0.14
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	16	0.14
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	16	0.14
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	16	0.14
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	16	0.14
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	16	0.14
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	16	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	5	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	6	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	7	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	8	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	12	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	14	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	16	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	17	0.14
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	18	0.14
(1,701)	1:55:A:LEU:HD21	1:55:A:LEU:H	1	0.14
(1,701)	1:55:A:LEU:HD22	1:55:A:LEU:H	1	0.14
(1,701)	1:55:A:LEU:HD23	1:55:A:LEU:H	1	0.14
(1,659)	1:46:A:LEU:HD21	1:46:A:LEU:H	14	0.14
(1,659)	1:46:A:LEU:HD22	1:46:A:LEU:H	14	0.14
(1,659)	1:46:A:LEU:HD23	1:46:A:LEU:H	14	0.14
(1,655)	1:42:A:VAL:HG21	1:100:A:ILE:H	8	0.14
(1,655)	1:42:A:VAL:HG22	1:100:A:ILE:H	8	0.14
(1,655)	1:42:A:VAL:HG23	1:100:A:ILE:H	8	0.14
(1,637)	1:42:A:VAL:HG21	1:99:A:MET:HA	17	0.14
(1,637)	1:42:A:VAL:HG22	1:99:A:MET:HA	17	0.14
(1,637)	1:42:A:VAL:HG23	1:99:A:MET:HA	17	0.14
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	18	0.14
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	18	0.14
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	18	0.14
(1,573)	1:33:A:LEU:HD11	1:33:A:LEU:H	2	0.14
(1,573)	1:33:A:LEU:HD12	1:33:A:LEU:H	2	0.14
(1,573)	1:33:A:LEU:HD13	1:33:A:LEU:H	2	0.14
(1,573)	1:33:A:LEU:HD11	1:33:A:LEU:H	9	0.14
(1,573)	1:33:A:LEU:HD12	1:33:A:LEU:H	9	0.14
(1,573)	1:33:A:LEU:HD13	1:33:A:LEU:H	9	0.14
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	8	0.14
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	8	0.14
(1,462)	1:8:A:SER:HB2	1:10:A:ASP:H	9	0.14
(1,462)	1:8:A:SER:HB3	1:10:A:ASP:H	9	0.14
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	17	0.14
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	17	0.14
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	17	0.14
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	20	0.14
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	20	0.14
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	20	0.14
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	11	0.14
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	11	0.14
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	11	0.14
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG12	11	0.14
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG13	11	0.14
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG12	11	0.14
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG13	11	0.14
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG12	19	0.14
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG13	19	0.14
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG12	19	0.14
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG13	19	0.14
(1,411)	1:99:A:MET:HE1	1:143:A:PHE:HB2	14	0.14
(1,411)	1:99:A:MET:HE1	1:143:A:PHE:HB3	14	0.14
(1,411)	1:99:A:MET:HE2	1:143:A:PHE:HB2	14	0.14
(1,411)	1:99:A:MET:HE2	1:143:A:PHE:HB3	14	0.14
(1,411)	1:99:A:MET:HE3	1:143:A:PHE:HB2	14	0.14
(1,411)	1:99:A:MET:HE3	1:143:A:PHE:HB3	14	0.14
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	3	0.14
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	3	0.14
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	9	0.14
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	9	0.14
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB1	8	0.14
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB2	8	0.14
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB3	8	0.14
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB1	8	0.14
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB2	8	0.14
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB3	8	0.14
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB2	5	0.14
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB3	5	0.14
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB2	5	0.14
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB3	5	0.14
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB2	5	0.14
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:33:A:LEU:HD11	1:39:A:VAL:HG21	9	0.14
(1,348)	1:33:A:LEU:HD11	1:39:A:VAL:HG22	9	0.14
(1,348)	1:33:A:LEU:HD11	1:39:A:VAL:HG23	9	0.14
(1,348)	1:33:A:LEU:HD12	1:39:A:VAL:HG21	9	0.14
(1,348)	1:33:A:LEU:HD12	1:39:A:VAL:HG22	9	0.14
(1,348)	1:33:A:LEU:HD12	1:39:A:VAL:HG23	9	0.14
(1,348)	1:33:A:LEU:HD13	1:39:A:VAL:HG21	9	0.14
(1,348)	1:33:A:LEU:HD13	1:39:A:VAL:HG22	9	0.14
(1,348)	1:33:A:LEU:HD13	1:39:A:VAL:HG23	9	0.14
(1,332)	1:150:A:LEU:HG	1:152:A:ASN:HB2	16	0.14
(1,332)	1:150:A:LEU:HG	1:152:A:ASN:HB3	16	0.14
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	8	0.14
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	13	0.14
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	20	0.14
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	20	0.14
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	20	0.14
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	17	0.14
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	17	0.14
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	17	0.14
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	17	0.14
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	17	0.14
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	17	0.14
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD1	2	0.14
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD2	2	0.14
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD1	2	0.14
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD2	2	0.14
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD1	9	0.14
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD2	9	0.14
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD1	9	0.14
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD2	9	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD21	14	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD22	14	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD23	14	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD21	14	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD22	14	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD23	14	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD21	14	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD22	14	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD23	14	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD21	16	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD22	16	0.14
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD23	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD21	16	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD22	16	0.14
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD23	16	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD21	16	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD22	16	0.14
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD23	16	0.14
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	1	0.14
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	1	0.14
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	1	0.14
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	1	0.14
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	1	0.14
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	1	0.14
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB2	11	0.14
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB3	11	0.14
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB2	11	0.14
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB3	11	0.14
(1,232)	1:92:A:ASN:HB2	1:93:A:LEU:HA	7	0.14
(1,232)	1:92:A:ASN:HB3	1:93:A:LEU:HA	7	0.14
(1,232)	1:92:A:ASN:HB2	1:93:A:LEU:HA	19	0.14
(1,232)	1:92:A:ASN:HB3	1:93:A:LEU:HA	19	0.14
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	8	0.14
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	8	0.14
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	8	0.14
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	15	0.14
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	15	0.14
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	15	0.14
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	2	0.14
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	2	0.14
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD1	4	0.14
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD2	4	0.14
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD1	5	0.14
(1,201)	1:120:A:LEU:HG	1:122:A:PHE:HD2	5	0.14
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	10	0.14
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	10	0.14
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	10	0.14
(1,183)	1:135:A:LEU:HD21	1:23:A:TRP:HH2	4	0.14
(1,183)	1:135:A:LEU:HD22	1:23:A:TRP:HH2	4	0.14
(1,183)	1:135:A:LEU:HD23	1:23:A:TRP:HH2	4	0.14
(1,164)	1:156:A:ILE:HD11	1:66:A:ASN:HA	10	0.14
(1,164)	1:156:A:ILE:HD12	1:66:A:ASN:HA	10	0.14
(1,164)	1:156:A:ILE:HD13	1:66:A:ASN:HA	10	0.14
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	19	0.14
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	19	0.14
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	19	0.14
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	19	0.14
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	19	0.14
(1,160)	1:156:A:ILE:HG21	1:153:A:ALA:HA	4	0.14
(1,160)	1:156:A:ILE:HG22	1:153:A:ALA:HA	4	0.14
(1,160)	1:156:A:ILE:HG23	1:153:A:ALA:HA	4	0.14
(1,160)	1:156:A:ILE:HG21	1:153:A:ALA:HA	5	0.14
(1,160)	1:156:A:ILE:HG22	1:153:A:ALA:HA	5	0.14
(1,160)	1:156:A:ILE:HG23	1:153:A:ALA:HA	5	0.14
(1,154)	1:162:A:THR:HG21	1:159:A:LEU:HA	5	0.14
(1,154)	1:162:A:THR:HG22	1:159:A:LEU:HA	5	0.14
(1,154)	1:162:A:THR:HG23	1:159:A:LEU:HA	5	0.14
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	4	0.14
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	4	0.14
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	4	0.14
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB1	17	0.14
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB2	17	0.14
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB3	17	0.14
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB1	17	0.14
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB2	17	0.14
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB3	17	0.14
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB1	17	0.14
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB2	17	0.14
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB3	17	0.14
(1,49)	1:150:A:LEU:HD11	1:64:A:ASP:HA	11	0.14
(1,49)	1:150:A:LEU:HD12	1:64:A:ASP:HA	11	0.14
(1,49)	1:150:A:LEU:HD13	1:64:A:ASP:HA	11	0.14
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD1	4	0.14
(1,41)	1:33:A:LEU:HD21	1:37:A:TYR:HD2	4	0.14
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD1	4	0.14
(1,41)	1:33:A:LEU:HD22	1:37:A:TYR:HD2	4	0.14
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD1	4	0.14
(1,41)	1:33:A:LEU:HD23	1:37:A:TYR:HD2	4	0.14
(1,39)	1:33:A:LEU:HD11	1:39:A:VAL:HG21	9	0.14
(1,39)	1:33:A:LEU:HD11	1:39:A:VAL:HG22	9	0.14
(1,39)	1:33:A:LEU:HD11	1:39:A:VAL:HG23	9	0.14
(1,39)	1:33:A:LEU:HD12	1:39:A:VAL:HG21	9	0.14
(1,39)	1:33:A:LEU:HD12	1:39:A:VAL:HG22	9	0.14
(1,39)	1:33:A:LEU:HD12	1:39:A:VAL:HG23	9	0.14
(1,39)	1:33:A:LEU:HD13	1:39:A:VAL:HG21	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:33:A:LEU:HD13	1:39:A:VAL:HG22	9	0.14
(1,39)	1:33:A:LEU:HD13	1:39:A:VAL:HG23	9	0.14
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	3	0.14
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	3	0.14
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	3	0.14
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	16	0.14
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	16	0.14
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	16	0.14
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD1	19	0.14
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD2	19	0.14
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD1	19	0.14
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD2	19	0.14
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD1	19	0.14
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD2	19	0.14
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD1	1	0.14
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD2	1	0.14
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD1	1	0.14
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD2	1	0.14
(1,13)	1:142:A:MET:HE1	1:94:A:LEU:HG	13	0.14
(1,13)	1:142:A:MET:HE2	1:94:A:LEU:HG	13	0.14
(1,13)	1:142:A:MET:HE3	1:94:A:LEU:HG	13	0.14
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD2	10	0.13
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD3	10	0.13
(1,2258)	1:137:A:ILE:HA	1:104:A:THR:H	2	0.13
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG21	1	0.13
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG22	1	0.13
(1,2197)	1:141:A:SER:H	1:100:A:ILE:HG23	1	0.13
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB1	16	0.13
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB2	16	0.13
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB3	16	0.13
(1,2170)	1:63:A:CYS:H	1:44:A:LYS:H	5	0.13
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	14	0.13
(1,2141)	1:65:A:ALA:HB1	1:67:A:TYR:H	5	0.13
(1,2141)	1:65:A:ALA:HB2	1:67:A:TYR:H	5	0.13
(1,2141)	1:65:A:ALA:HB3	1:67:A:TYR:H	5	0.13
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	4	0.13
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	4	0.13
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	4	0.13
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	16	0.13
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	16	0.13
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	16	0.13
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	7	0.13
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	9	0.13
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	20	0.13
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	6	0.13
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	12	0.13
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	20	0.13
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	20	0.13
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	6	0.13
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	6	0.13
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	12	0.13
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	12	0.13
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	19	0.13
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	19	0.13
(1,2045)	1:73:A:ALA:H	1:137:A:ILE:HB	16	0.13
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG11	20	0.13
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG12	20	0.13
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG13	20	0.13
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	1	0.13
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	3	0.13
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	7	0.13
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	13	0.13
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	14	0.13
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	15	0.13
(1,2004)	1:78:A:ILE:H	1:140:A:PHE:HE1	9	0.13
(1,2004)	1:78:A:ILE:H	1:140:A:PHE:HE2	9	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	3	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	3	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	3	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	18	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	18	0.13
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	18	0.13
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD11	18	0.13
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD12	18	0.13
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD13	18	0.13
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD1	14	0.13
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD2	14	0.13
(1,1820)	1:175:A:SER:H	1:174:A:PHE:H	8	0.13
(1,1790)	1:91:A:GLN:HG2	1:91:A:GLN:H	17	0.13
(1,1790)	1:91:A:GLN:HG3	1:91:A:GLN:H	17	0.13
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	8	0.13
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	8	0.13
(1,1759)	1:54:A:THR:HB	1:55:A:LEU:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1759)	1:54:A:THR:HB	1:55:A:LEU:H	12	0.13
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD11	10	0.13
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD12	10	0.13
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD13	10	0.13
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	8	0.13
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	9	0.13
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB2	1	0.13
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB3	1	0.13
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	9	0.13
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	6	0.13
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	12	0.13
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	4	0.13
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	5	0.13
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	8	0.13
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	15	0.13
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	19	0.13
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	13	0.13
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	14	0.13
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	15	0.13
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	20	0.13
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	2	0.13
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	3	0.13
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	5	0.13
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	17	0.13
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	18	0.13
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	19	0.13
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	14	0.13
(1,1442)	1:175:A:SER:HB2	1:175:A:SER:H	7	0.13
(1,1442)	1:175:A:SER:HB3	1:175:A:SER:H	7	0.13
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG2	14	0.13
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG3	14	0.13
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	14	0.13
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	14	0.13
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	14	0.13
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	14	0.13
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	14	0.13
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	14	0.13
(1,1348)	1:159:A:LEU:HD21	1:159:A:LEU:H	15	0.13
(1,1348)	1:159:A:LEU:HD22	1:159:A:LEU:H	15	0.13
(1,1348)	1:159:A:LEU:HD23	1:159:A:LEU:H	15	0.13
(1,1342)	1:159:A:LEU:HA	1:159:A:LEU:HD21	11	0.13
(1,1342)	1:159:A:LEU:HA	1:159:A:LEU:HD22	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1342)	1:159:A:LEU:HA	1:159:A:LEU:HD23	11	0.13
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG21	13	0.13
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG22	13	0.13
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG23	13	0.13
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG21	13	0.13
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG22	13	0.13
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG23	13	0.13
(1,1266)	1:142:A:MET:HE1	1:97:A:GLU:H	11	0.13
(1,1266)	1:142:A:MET:HE2	1:97:A:GLU:H	11	0.13
(1,1266)	1:142:A:MET:HE3	1:97:A:GLU:H	11	0.13
(1,1266)	1:142:A:MET:HE1	1:97:A:GLU:H	13	0.13
(1,1266)	1:142:A:MET:HE2	1:97:A:GLU:H	13	0.13
(1,1266)	1:142:A:MET:HE3	1:97:A:GLU:H	13	0.13
(1,1248)	1:140:A:PHE:HA	1:102:A:SER:H	6	0.13
(1,1248)	1:140:A:PHE:HA	1:102:A:SER:H	12	0.13
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	16	0.13
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	16	0.13
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	16	0.13
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	4	0.13
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	4	0.13
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	4	0.13
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	18	0.13
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	18	0.13
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	18	0.13
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	2	0.13
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	2	0.13
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	2	0.13
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD21	18	0.13
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD22	18	0.13
(1,1157)	1:128:A:LEU:HA	1:128:A:LEU:HD23	18	0.13
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	15	0.13
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	1	0.13
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	1	0.13
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	1	0.13
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	1	0.13
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	1	0.13
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	1	0.13
(1,1107)	1:113:A:VAL:HG21	1:114:A:GLN:HE22	1	0.13
(1,1107)	1:113:A:VAL:HG22	1:114:A:GLN:HE22	1	0.13
(1,1107)	1:113:A:VAL:HG23	1:114:A:GLN:HE22	1	0.13
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	5	0.13
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	11	0.13
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	13	0.13
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	17	0.13
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	18	0.13
(1,1077)	1:107:A:PHE:HA	1:134:A:VAL:H	2	0.13
(1,1029)	1:100:A:ILE:HD11	1:23:A:TRP:HZ2	19	0.13
(1,1029)	1:100:A:ILE:HD12	1:23:A:TRP:HZ2	19	0.13
(1,1029)	1:100:A:ILE:HD13	1:23:A:TRP:HZ2	19	0.13
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	14	0.13
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	14	0.13
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	14	0.13
(1,973)	1:94:A:LEU:HD21	1:94:A:LEU:H	17	0.13
(1,973)	1:94:A:LEU:HD22	1:94:A:LEU:H	17	0.13
(1,973)	1:94:A:LEU:HD23	1:94:A:LEU:H	17	0.13
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	1	0.13
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	1	0.13
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	18	0.13
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	18	0.13
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	19	0.13
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	19	0.13
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	20	0.13
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	20	0.13
(1,862)	1:74:A:ASN:HB2	1:138:A:ASN:HD21	5	0.13
(1,862)	1:74:A:ASN:HB3	1:138:A:ASN:HD21	5	0.13
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	9	0.13
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	9	0.13
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	9	0.13
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	9	0.13
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	9	0.13
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	9	0.13
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	20	0.13
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	20	0.13
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	20	0.13
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	20	0.13
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	20	0.13
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	20	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	8	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	8	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	8	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	8	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	8	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	8	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	8	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	8	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	9	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	9	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	9	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	9	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	9	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	9	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	9	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	9	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	9	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	17	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	17	0.13
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	17	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	17	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	17	0.13
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	17	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	17	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	17	0.13
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	17	0.13
(1,756)	1:64:A:ASP:HA	1:23:A:TRP:HE1	5	0.13
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	2	0.13
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	15	0.13
(1,703)	1:55:A:LEU:HG	1:55:A:LEU:H	16	0.13
(1,701)	1:55:A:LEU:HD21	1:55:A:LEU:H	2	0.13
(1,701)	1:55:A:LEU:HD22	1:55:A:LEU:H	2	0.13
(1,701)	1:55:A:LEU:HD23	1:55:A:LEU:H	2	0.13
(1,701)	1:55:A:LEU:HD21	1:55:A:LEU:H	17	0.13
(1,701)	1:55:A:LEU:HD22	1:55:A:LEU:H	17	0.13
(1,701)	1:55:A:LEU:HD23	1:55:A:LEU:H	17	0.13
(1,680)	1:48:A:ILE:HD11	1:90:A:THR:HA	2	0.13
(1,680)	1:48:A:ILE:HD12	1:90:A:THR:HA	2	0.13
(1,680)	1:48:A:ILE:HD13	1:90:A:THR:HA	2	0.13
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	11	0.13
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	11	0.13
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	11	0.13
(1,631)	1:42:A:VAL:HG11	1:143:A:PHE:HD1	4	0.13
(1,631)	1:42:A:VAL:HG11	1:143:A:PHE:HD2	4	0.13
(1,631)	1:42:A:VAL:HG12	1:143:A:PHE:HD1	4	0.13
(1,631)	1:42:A:VAL:HG12	1:143:A:PHE:HD2	4	0.13
(1,631)	1:42:A:VAL:HG13	1:143:A:PHE:HD1	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:42:A:VAL:HG13	1:143:A:PHE:HD2	4	0.13
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB2	8	0.13
(1,629)	1:45:A:VAL:HG21	1:94:A:LEU:HB3	8	0.13
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB2	8	0.13
(1,629)	1:45:A:VAL:HG22	1:94:A:LEU:HB3	8	0.13
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB2	8	0.13
(1,629)	1:45:A:VAL:HG23	1:94:A:LEU:HB3	8	0.13
(1,615)	1:41:A:LYS:HD2	1:41:A:LYS:HA	18	0.13
(1,615)	1:41:A:LYS:HD3	1:41:A:LYS:HA	18	0.13
(1,614)	1:41:A:LYS:HA	1:41:A:LYS:HD2	18	0.13
(1,614)	1:41:A:LYS:HA	1:41:A:LYS:HD3	18	0.13
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD1	19	0.13
(1,583)	1:37:A:TYR:HA	1:37:A:TYR:HD2	19	0.13
(1,573)	1:33:A:LEU:HD11	1:33:A:LEU:H	15	0.13
(1,573)	1:33:A:LEU:HD12	1:33:A:LEU:H	15	0.13
(1,573)	1:33:A:LEU:HD13	1:33:A:LEU:H	15	0.13
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	15	0.13
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	15	0.13
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	15	0.13
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	16	0.13
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	16	0.13
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	16	0.13
(1,520)	1:24:A:LEU:HD21	1:23:A:TRP:HZ2	5	0.13
(1,520)	1:24:A:LEU:HD22	1:23:A:TRP:HZ2	5	0.13
(1,520)	1:24:A:LEU:HD23	1:23:A:TRP:HZ2	5	0.13
(1,506)	1:23:A:TRP:HD1	1:23:A:TRP:HA	18	0.13
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	2	0.13
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	2	0.13
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	2	0.13
(1,481)	1:14:A:VAL:HG11	1:15:A:THR:H	13	0.13
(1,481)	1:14:A:VAL:HG12	1:15:A:THR:H	13	0.13
(1,481)	1:14:A:VAL:HG13	1:15:A:THR:H	13	0.13
(1,478)	1:12:A:VAL:HG11	1:12:A:VAL:H	14	0.13
(1,478)	1:12:A:VAL:HG12	1:12:A:VAL:H	14	0.13
(1,478)	1:12:A:VAL:HG13	1:12:A:VAL:H	14	0.13
(1,462)	1:8:A:SER:HB2	1:10:A:ASP:H	19	0.13
(1,462)	1:8:A:SER:HB3	1:10:A:ASP:H	19	0.13
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	11	0.13
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	11	0.13
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	11	0.13
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	6	0.13
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	6	0.13
(1,449)	1:170:A:ILE:HG21	1:166:A:ILE:HA	12	0.13
(1,449)	1:170:A:ILE:HG22	1:166:A:ILE:HA	12	0.13
(1,449)	1:170:A:ILE:HG23	1:166:A:ILE:HA	12	0.13
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG21	19	0.13
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG22	19	0.13
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG23	19	0.13
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG21	19	0.13
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG22	19	0.13
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG23	19	0.13
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	5	0.13
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	5	0.13
(1,388)	1:85:A:GLU:HA	1:87:A:ARG:H	15	0.13
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB1	20	0.13
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB2	20	0.13
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB3	20	0.13
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB1	20	0.13
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB2	20	0.13
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB3	20	0.13
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	8	0.13
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	8	0.13
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	8	0.13
(1,385)	1:78:A:ILE:HG21	1:57:A:SER:HA	9	0.13
(1,385)	1:78:A:ILE:HG22	1:57:A:SER:HA	9	0.13
(1,385)	1:78:A:ILE:HG23	1:57:A:SER:HA	9	0.13
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD11	14	0.13
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD12	14	0.13
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD13	14	0.13
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD11	14	0.13
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD12	14	0.13
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD13	14	0.13
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD11	14	0.13
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD12	14	0.13
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD13	14	0.13
(1,346)	1:31:A:ALA:HB1	1:26:A:PRO:HB2	14	0.13
(1,346)	1:31:A:ALA:HB1	1:26:A:PRO:HB3	14	0.13
(1,346)	1:31:A:ALA:HB2	1:26:A:PRO:HB2	14	0.13
(1,346)	1:31:A:ALA:HB2	1:26:A:PRO:HB3	14	0.13
(1,346)	1:31:A:ALA:HB3	1:26:A:PRO:HB2	14	0.13
(1,346)	1:31:A:ALA:HB3	1:26:A:PRO:HB3	14	0.13
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	2	0.13
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:172:A:GLN:HG2	1:170:A:ILE:HA	7	0.13
(1,313)	1:172:A:GLN:HG3	1:170:A:ILE:HA	7	0.13
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	3	0.13
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	3	0.13
(1,298)	1:24:A:LEU:HD11	1:69:A:ILE:H	4	0.13
(1,298)	1:24:A:LEU:HD12	1:69:A:ILE:H	4	0.13
(1,298)	1:24:A:LEU:HD13	1:69:A:ILE:H	4	0.13
(1,281)	1:42:A:VAL:HB	1:20:A:MET:HG2	17	0.13
(1,281)	1:42:A:VAL:HB	1:20:A:MET:HG3	17	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	4	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	4	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	4	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	9	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	9	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	9	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	19	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	19	0.13
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	19	0.13
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	1	0.13
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	1	0.13
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	1	0.13
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	9	0.13
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	9	0.13
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	9	0.13
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG21	11	0.13
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG22	11	0.13
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG23	11	0.13
(1,251)	1:76:A:LYS:HG2	1:74:A:ASN:HD21	13	0.13
(1,251)	1:76:A:LYS:HG2	1:74:A:ASN:HD22	13	0.13
(1,251)	1:76:A:LYS:HG3	1:74:A:ASN:HD21	13	0.13
(1,251)	1:76:A:LYS:HG3	1:74:A:ASN:HD22	13	0.13
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	2	0.13
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	2	0.13
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	2	0.13
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	2	0.13
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	2	0.13
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	2	0.13
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	7	0.13
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	7	0.13
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	7	0.13
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	7	0.13
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	7	0.13
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB2	6	0.13
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB3	6	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB2	6	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB3	6	0.13
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB2	10	0.13
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB3	10	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB2	10	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB3	10	0.13
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB2	12	0.13
(1,235)	1:9:A:ARG:HD2	1:8:A:SER:HB3	12	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB2	12	0.13
(1,235)	1:9:A:ARG:HD3	1:8:A:SER:HB3	12	0.13
(1,232)	1:92:A:ASN:HB2	1:93:A:LEU:HA	2	0.13
(1,232)	1:92:A:ASN:HB3	1:93:A:LEU:HA	2	0.13
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	10	0.13
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	10	0.13
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	5	0.13
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	5	0.13
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	5	0.13
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	18	0.13
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	18	0.13
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	18	0.13
(1,174)	1:149:A:ILE:HG12	1:95:A:ASN:HD22	8	0.13
(1,174)	1:149:A:ILE:HG13	1:95:A:ASN:HD22	8	0.13
(1,160)	1:156:A:ILE:HG21	1:153:A:ALA:HA	11	0.13
(1,160)	1:156:A:ILE:HG22	1:153:A:ALA:HA	11	0.13
(1,160)	1:156:A:ILE:HG23	1:153:A:ALA:HA	11	0.13
(1,160)	1:156:A:ILE:HG21	1:153:A:ALA:HA	16	0.13
(1,160)	1:156:A:ILE:HG22	1:153:A:ALA:HA	16	0.13
(1,160)	1:156:A:ILE:HG23	1:153:A:ALA:HA	16	0.13
(1,155)	1:162:A:THR:HG21	1:67:A:TYR:HB2	13	0.13
(1,155)	1:162:A:THR:HG21	1:67:A:TYR:HB3	13	0.13
(1,155)	1:162:A:THR:HG22	1:67:A:TYR:HB2	13	0.13
(1,155)	1:162:A:THR:HG22	1:67:A:TYR:HB3	13	0.13
(1,155)	1:162:A:THR:HG23	1:67:A:TYR:HB2	13	0.13
(1,155)	1:162:A:THR:HG23	1:67:A:TYR:HB3	13	0.13
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	9	0.13
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	9	0.13
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	9	0.13
(1,150)	1:166:A:ILE:HG21	1:170:A:ILE:H	17	0.13
(1,150)	1:166:A:ILE:HG22	1:170:A:ILE:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:166:A:ILE:HG23	1:170:A:ILE:H	17	0.13
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	5	0.13
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	5	0.13
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	5	0.13
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB1	18	0.13
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB2	18	0.13
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB3	18	0.13
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB1	18	0.13
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB2	18	0.13
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB3	18	0.13
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB1	18	0.13
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB2	18	0.13
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB3	18	0.13
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	6	0.13
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	6	0.13
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	6	0.13
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	12	0.13
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	12	0.13
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	12	0.13
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE1	6	0.13
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE2	6	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE1	6	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE2	6	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE1	6	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE2	6	0.13
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE1	12	0.13
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE2	12	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE1	12	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE2	12	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE1	12	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE2	12	0.13
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE1	16	0.13
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE2	16	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE1	16	0.13
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE2	16	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE1	16	0.13
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE2	16	0.13
(1,54)	1:23:A:TRP:H	1:24:A:LEU:H	18	0.13
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	3	0.13
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	3	0.13
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	3	0.13
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	4	0.13
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	4	0.13
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	8	0.13
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	8	0.13
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	8	0.13
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	16	0.13
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	16	0.13
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	16	0.13
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG21	9	0.13
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG22	9	0.13
(1,38)	1:33:A:LEU:HD11	1:27:A:VAL:HG23	9	0.13
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG21	9	0.13
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG22	9	0.13
(1,38)	1:33:A:LEU:HD12	1:27:A:VAL:HG23	9	0.13
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG21	9	0.13
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG22	9	0.13
(1,38)	1:33:A:LEU:HD13	1:27:A:VAL:HG23	9	0.13
(1,34)	1:39:A:VAL:HG11	1:37:A:TYR:HD1	18	0.13
(1,34)	1:39:A:VAL:HG11	1:37:A:TYR:HD2	18	0.13
(1,34)	1:39:A:VAL:HG12	1:37:A:TYR:HD1	18	0.13
(1,34)	1:39:A:VAL:HG12	1:37:A:TYR:HD2	18	0.13
(1,34)	1:39:A:VAL:HG13	1:37:A:TYR:HD1	18	0.13
(1,34)	1:39:A:VAL:HG13	1:37:A:TYR:HD2	18	0.13
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD1	20	0.13
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD2	20	0.13
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD1	20	0.13
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD2	20	0.13
(1,8)	1:96:A:SER:HA	1:147:A:GLN:HG2	9	0.13
(1,8)	1:96:A:SER:HA	1:147:A:GLN:HG3	9	0.13
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD2	1	0.12
(1,2262)	1:89:A:VAL:H	1:88:A:ARG:HD3	1	0.12
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD11	1	0.12
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD12	1	0.12
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD13	1	0.12
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD11	7	0.12
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD12	7	0.12
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD13	7	0.12
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD11	17	0.12
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD12	17	0.12
(1,2244)	1:23:A:TRP:HE1	1:100:A:ILE:HD13	17	0.12
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB1	14	0.12
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB3	14	0.12
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	8	0.12
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	16	0.12
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG21	3	0.12
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG22	3	0.12
(1,2182)	1:158:A:PHE:H	1:156:A:ILE:HG23	3	0.12
(1,2180)	1:140:A:PHE:HD1	1:142:A:MET:H	5	0.12
(1,2180)	1:140:A:PHE:HD2	1:142:A:MET:H	5	0.12
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	15	0.12
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	18	0.12
(1,2141)	1:65:A:ALA:HB1	1:67:A:TYR:H	14	0.12
(1,2141)	1:65:A:ALA:HB2	1:67:A:TYR:H	14	0.12
(1,2141)	1:65:A:ALA:HB3	1:67:A:TYR:H	14	0.12
(1,2120)	1:37:A:TYR:H	1:37:A:TYR:HD1	18	0.12
(1,2120)	1:37:A:TYR:H	1:37:A:TYR:HD2	18	0.12
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	4	0.12
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	14	0.12
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	17	0.12
(1,2096)	1:109:A:ASN:H	1:112:A:GLN:HA	14	0.12
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE1	14	0.12
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE2	14	0.12
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG21	20	0.12
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG22	20	0.12
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG23	20	0.12
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	14	0.12
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	14	0.12
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG11	5	0.12
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG12	5	0.12
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG13	5	0.12
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	4	0.12
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	16	0.12
(1,1918)	1:13:A:ARG:H	1:12:A:VAL:HB	6	0.12
(1,1918)	1:13:A:ARG:H	1:12:A:VAL:HB	12	0.12
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	20	0.12
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	20	0.12
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	8	0.12
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	8	0.12
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	8	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD11	1	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD12	1	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD13	1	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD11	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD12	5	0.12
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD13	5	0.12
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD1	16	0.12
(1,1845)	1:81:A:PHE:H	1:81:A:PHE:HD2	16	0.12
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD1	16	0.12
(1,1773)	1:49:A:TYR:H	1:49:A:TYR:HD2	16	0.12
(1,1765)	1:11:A:ALA:H	1:10:A:ASP:H	15	0.12
(1,1761)	1:55:A:LEU:H	1:56:A:SER:HA	2	0.12
(1,1759)	1:54:A:THR:HB	1:55:A:LEU:H	9	0.12
(1,1759)	1:54:A:THR:HB	1:55:A:LEU:H	13	0.12
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB2	1	0.12
(1,1748)	1:55:A:LEU:H	1:56:A:SER:HB3	1	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD11	17	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD12	17	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD13	17	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD11	18	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD12	18	0.12
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD13	18	0.12
(1,1726)	1:166:A:ILE:HA	1:171:A:GLU:H	9	0.12
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	1	0.12
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	10	0.12
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	6	0.12
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	6	0.12
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	12	0.12
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	12	0.12
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	7	0.12
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	7	0.12
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	7	0.12
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	14	0.12
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	14	0.12
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	14	0.12
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	19	0.12
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	19	0.12
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	19	0.12
(1,1681)	1:170:A:ILE:H	1:167:A:ALA:HA	4	0.12
(1,1681)	1:170:A:ILE:H	1:167:A:ALA:HA	10	0.12
(1,1640)	1:86:A:ARG:H	1:86:A:ARG:HG2	19	0.12
(1,1640)	1:86:A:ARG:H	1:86:A:ARG:HG3	19	0.12
(1,1633)	1:156:A:ILE:HB	1:155:A:THR:H	5	0.12
(1,1633)	1:156:A:ILE:HB	1:155:A:THR:H	13	0.12
(1,1633)	1:156:A:ILE:HB	1:155:A:THR:H	14	0.12
(1,1601)	1:102:A:SER:H	1:137:A:ILE:HG21	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1601)	1:102:A:SER:H	1:137:A:ILE:HG22	5	0.12
(1,1601)	1:102:A:SER:H	1:137:A:ILE:HG23	5	0.12
(1,1596)	1:102:A:SER:H	1:101:A:HIS:HD2	10	0.12
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	5	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	3	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	7	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	9	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	10	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	13	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	16	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	17	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	18	0.12
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	20	0.12
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	1	0.12
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	7	0.12
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	8	0.12
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	4	0.12
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	9	0.12
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	10	0.12
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	14	0.12
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	6	0.12
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	12	0.12
(1,1486)	1:124:A:GLN:HE22	1:129:A:PHE:HA	11	0.12
(1,1482)	1:121:A:LYS:HE2	1:114:A:GLN:HE22	3	0.12
(1,1482)	1:121:A:LYS:HE3	1:114:A:GLN:HE22	3	0.12
(1,1481)	1:124:A:GLN:HE22	1:129:A:PHE:HE1	6	0.12
(1,1481)	1:124:A:GLN:HE22	1:129:A:PHE:HE2	6	0.12
(1,1481)	1:124:A:GLN:HE22	1:129:A:PHE:HE1	12	0.12
(1,1481)	1:124:A:GLN:HE22	1:129:A:PHE:HE2	12	0.12
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG2	4	0.12
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG3	4	0.12
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	5	0.12
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	5	0.12
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	5	0.12
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	5	0.12
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	5	0.12
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	5	0.12
(1,1310)	1:156:A:ILE:HB	1:157:A:GLU:H	6	0.12
(1,1310)	1:156:A:ILE:HB	1:157:A:GLU:H	12	0.12
(1,1310)	1:156:A:ILE:HB	1:157:A:GLU:H	16	0.12
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG21	10	0.12
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG22	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG23	10	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG21	10	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG22	10	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG23	10	0.12
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG21	19	0.12
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG22	19	0.12
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG23	19	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG21	19	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG22	19	0.12
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG23	19	0.12
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	11	0.12
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	11	0.12
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	11	0.12
(1,1248)	1:140:A:PHE:HA	1:102:A:SER:H	20	0.12
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	3	0.12
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	3	0.12
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	3	0.12
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	13	0.12
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	13	0.12
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	13	0.12
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	20	0.12
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	20	0.12
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	20	0.12
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	2	0.12
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	2	0.12
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	2	0.12
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	3	0.12
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	3	0.12
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	3	0.12
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	10	0.12
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	10	0.12
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	10	0.12
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	16	0.12
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	16	0.12
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	16	0.12
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	6	0.12
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	6	0.12
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	6	0.12
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	12	0.12
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	12	0.12
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	12	0.12
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	17	0.12
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	17	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	6	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	6	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	6	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	12	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	12	0.12
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	12	0.12
(1,1159)	1:109:A:ASN:HB2	1:130:A:PRO:HA	6	0.12
(1,1159)	1:109:A:ASN:HB3	1:130:A:PRO:HA	6	0.12
(1,1159)	1:109:A:ASN:HB2	1:130:A:PRO:HA	12	0.12
(1,1159)	1:109:A:ASN:HB3	1:130:A:PRO:HA	12	0.12
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	6	0.12
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	6	0.12
(1,1152)	1:125:A:LYS:HB2	1:125:A:LYS:H	12	0.12
(1,1152)	1:125:A:LYS:HB3	1:125:A:LYS:H	12	0.12
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	13	0.12
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	13	0.12
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	13	0.12
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	13	0.12
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	13	0.12
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	13	0.12
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	7	0.12
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	7	0.12
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	7	0.12
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	7	0.12
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	7	0.12
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	7	0.12
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	7	0.12
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	7	0.12
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	7	0.12
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	13	0.12
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	13	0.12
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	13	0.12
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	13	0.12
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	13	0.12
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	13	0.12
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	13	0.12
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	13	0.12
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	13	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	1	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	3	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	4	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	8	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	9	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	10	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	14	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	16	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	19	0.12
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	20	0.12
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD1	17	0.12
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD2	17	0.12
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD1	17	0.12
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD2	17	0.12
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD1	17	0.12
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD2	17	0.12
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD1	19	0.12
(1,1030)	1:100:A:ILE:HD11	1:103:A:PHE:HD2	19	0.12
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD1	19	0.12
(1,1030)	1:100:A:ILE:HD12	1:103:A:PHE:HD2	19	0.12
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD1	19	0.12
(1,1030)	1:100:A:ILE:HD13	1:103:A:PHE:HD2	19	0.12
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	9	0.12
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	9	0.12
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	9	0.12
(1,1018)	1:99:A:MET:HG2	1:100:A:ILE:H	9	0.12
(1,1018)	1:99:A:MET:HG3	1:100:A:ILE:H	9	0.12
(1,1018)	1:99:A:MET:HG2	1:100:A:ILE:H	14	0.12
(1,1018)	1:99:A:MET:HG3	1:100:A:ILE:H	14	0.12
(1,1016)	1:99:A:MET:HE1	1:143:A:PHE:HZ	3	0.12
(1,1016)	1:99:A:MET:HE2	1:143:A:PHE:HZ	3	0.12
(1,1016)	1:99:A:MET:HE3	1:143:A:PHE:HZ	3	0.12
(1,1012)	1:99:A:MET:HE1	1:99:A:MET:HA	3	0.12
(1,1012)	1:99:A:MET:HE2	1:99:A:MET:HA	3	0.12
(1,1012)	1:99:A:MET:HE3	1:99:A:MET:HA	3	0.12
(1,1012)	1:99:A:MET:HE1	1:99:A:MET:HA	4	0.12
(1,1012)	1:99:A:MET:HE2	1:99:A:MET:HA	4	0.12
(1,1012)	1:99:A:MET:HE3	1:99:A:MET:HA	4	0.12
(1,1012)	1:99:A:MET:HE1	1:99:A:MET:HA	8	0.12
(1,1012)	1:99:A:MET:HE2	1:99:A:MET:HA	8	0.12
(1,1012)	1:99:A:MET:HE3	1:99:A:MET:HA	8	0.12
(1,974)	1:45:A:VAL:HG21	1:95:A:ASN:H	11	0.12
(1,974)	1:45:A:VAL:HG22	1:95:A:ASN:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:45:A:VAL:HG23	1:95:A:ASN:H	11	0.12
(1,951)	1:89:A:VAL:HG21	1:140:A:PHE:HZ	8	0.12
(1,951)	1:89:A:VAL:HG22	1:140:A:PHE:HZ	8	0.12
(1,951)	1:89:A:VAL:HG23	1:140:A:PHE:HZ	8	0.12
(1,951)	1:89:A:VAL:HG21	1:140:A:PHE:HZ	10	0.12
(1,951)	1:89:A:VAL:HG22	1:140:A:PHE:HZ	10	0.12
(1,951)	1:89:A:VAL:HG23	1:140:A:PHE:HZ	10	0.12
(1,922)	1:83:A:ARG:HA	1:83:A:ARG:HD2	5	0.12
(1,922)	1:83:A:ARG:HA	1:83:A:ARG:HD3	5	0.12
(1,886)	1:77:A:ALA:HB1	1:138:A:ASN:HA	5	0.12
(1,886)	1:77:A:ALA:HB2	1:138:A:ASN:HA	5	0.12
(1,886)	1:77:A:ALA:HB3	1:138:A:ASN:HA	5	0.12
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	11	0.12
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	11	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD11	16	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD12	16	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD13	16	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD11	17	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD12	17	0.12
(1,856)	1:74:A:ASN:HA	1:78:A:ILE:HD13	17	0.12
(1,854)	1:73:A:ALA:HB1	1:140:A:PHE:HZ	8	0.12
(1,854)	1:73:A:ALA:HB2	1:140:A:PHE:HZ	8	0.12
(1,854)	1:73:A:ALA:HB3	1:140:A:PHE:HZ	8	0.12
(1,854)	1:73:A:ALA:HB1	1:140:A:PHE:HZ	13	0.12
(1,854)	1:73:A:ALA:HB2	1:140:A:PHE:HZ	13	0.12
(1,854)	1:73:A:ALA:HB3	1:140:A:PHE:HZ	13	0.12
(1,822)	1:70:A:LEU:HD21	1:113:A:VAL:HA	6	0.12
(1,822)	1:70:A:LEU:HD22	1:113:A:VAL:HA	6	0.12
(1,822)	1:70:A:LEU:HD23	1:113:A:VAL:HA	6	0.12
(1,822)	1:70:A:LEU:HD21	1:113:A:VAL:HA	12	0.12
(1,822)	1:70:A:LEU:HD22	1:113:A:VAL:HA	12	0.12
(1,822)	1:70:A:LEU:HD23	1:113:A:VAL:HA	12	0.12
(1,822)	1:70:A:LEU:HD21	1:113:A:VAL:HA	18	0.12
(1,822)	1:70:A:LEU:HD22	1:113:A:VAL:HA	18	0.12
(1,822)	1:70:A:LEU:HD23	1:113:A:VAL:HA	18	0.12
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	4	0.12
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	4	0.12
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	4	0.12
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	4	0.12
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	4	0.12
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	4	0.12
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	4	0.12
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	4	0.12
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD21	5	0.12
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD22	5	0.12
(1,794)	1:69:A:ILE:HD11	1:24:A:LEU:HD23	5	0.12
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD21	5	0.12
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD22	5	0.12
(1,794)	1:69:A:ILE:HD12	1:24:A:LEU:HD23	5	0.12
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD21	5	0.12
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD22	5	0.12
(1,794)	1:69:A:ILE:HD13	1:24:A:LEU:HD23	5	0.12
(1,756)	1:64:A:ASP:HA	1:23:A:TRP:HE1	4	0.12
(1,748)	1:62:A:LEU:HD11	1:45:A:VAL:HA	13	0.12
(1,748)	1:62:A:LEU:HD12	1:45:A:VAL:HA	13	0.12
(1,748)	1:62:A:LEU:HD13	1:45:A:VAL:HA	13	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	11	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	11	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	11	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	11	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	11	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	11	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	11	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	11	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	11	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	15	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	15	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	15	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	15	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	15	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	15	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	15	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	15	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	15	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	16	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	16	0.12
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	16	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	16	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	16	0.12
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	16	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	16	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	16	0.12
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:48:A:ILE:HA	1:60:A:LEU:HA	17	0.12
(1,704)	1:55:A:LEU:HG	1:55:A:LEU:HA	10	0.12
(1,680)	1:48:A:ILE:HD11	1:90:A:THR:HA	16	0.12
(1,680)	1:48:A:ILE:HD12	1:90:A:THR:HA	16	0.12
(1,680)	1:48:A:ILE:HD13	1:90:A:THR:HA	16	0.12
(1,644)	1:24:A:LEU:HD21	1:43:A:LEU:HD11	18	0.12
(1,644)	1:24:A:LEU:HD21	1:43:A:LEU:HD12	18	0.12
(1,644)	1:24:A:LEU:HD21	1:43:A:LEU:HD13	18	0.12
(1,644)	1:24:A:LEU:HD22	1:43:A:LEU:HD11	18	0.12
(1,644)	1:24:A:LEU:HD22	1:43:A:LEU:HD12	18	0.12
(1,644)	1:24:A:LEU:HD22	1:43:A:LEU:HD13	18	0.12
(1,644)	1:24:A:LEU:HD23	1:43:A:LEU:HD11	18	0.12
(1,644)	1:24:A:LEU:HD23	1:43:A:LEU:HD12	18	0.12
(1,644)	1:24:A:LEU:HD23	1:43:A:LEU:HD13	18	0.12
(1,601)	1:39:A:VAL:HG11	1:39:A:VAL:H	9	0.12
(1,601)	1:39:A:VAL:HG12	1:39:A:VAL:H	9	0.12
(1,601)	1:39:A:VAL:HG13	1:39:A:VAL:H	9	0.12
(1,587)	1:38:A:LYS:HA	1:102:A:SER:HA	11	0.12
(1,575)	1:33:A:LEU:HG	1:33:A:LEU:H	11	0.12
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	8	0.12
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	8	0.12
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	8	0.12
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	19	0.12
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	19	0.12
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	19	0.12
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	7	0.12
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	7	0.12
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	7	0.12
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	14	0.12
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	14	0.12
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	14	0.12
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	20	0.12
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	20	0.12
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	20	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG21	6	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG22	6	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG23	6	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG21	6	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG22	6	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG23	6	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG21	6	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG22	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG23	6	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG21	12	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG22	12	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG23	12	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG21	12	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG22	12	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG23	12	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG21	12	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG22	12	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG23	12	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG21	14	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG22	14	0.12
(1,498)	1:20:A:MET:HE1	1:42:A:VAL:HG23	14	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG21	14	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG22	14	0.12
(1,498)	1:20:A:MET:HE2	1:42:A:VAL:HG23	14	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG21	14	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG22	14	0.12
(1,498)	1:20:A:MET:HE3	1:42:A:VAL:HG23	14	0.12
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	7	0.12
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	7	0.12
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	7	0.12
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	6	0.12
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	6	0.12
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	6	0.12
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	12	0.12
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	12	0.12
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	12	0.12
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	13	0.12
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	13	0.12
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	13	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	5	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	5	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	5	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	5	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	5	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	5	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	10	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	10	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	10	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	10	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	10	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	13	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	13	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	13	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	13	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	13	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	13	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	14	0.12
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	14	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	14	0.12
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	14	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	14	0.12
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	14	0.12
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD1	7	0.12
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD2	7	0.12
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD1	7	0.12
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD2	7	0.12
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD1	7	0.12
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD2	7	0.12
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD1	17	0.12
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD2	17	0.12
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD1	17	0.12
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD2	17	0.12
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD1	17	0.12
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD2	17	0.12
(1,412)	1:137:A:ILE:HD11	1:71:A:ALA:H	18	0.12
(1,412)	1:137:A:ILE:HD12	1:71:A:ALA:H	18	0.12
(1,412)	1:137:A:ILE:HD13	1:71:A:ALA:H	18	0.12
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB2	19	0.12
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB3	19	0.12
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB2	19	0.12
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB3	19	0.12
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB2	19	0.12
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB3	19	0.12
(1,341)	1:20:A:MET:HE1	1:66:A:ASN:H	8	0.12
(1,341)	1:20:A:MET:HE2	1:66:A:ASN:H	8	0.12
(1,341)	1:20:A:MET:HE3	1:66:A:ASN:H	8	0.12
(1,334)	1:26:A:PRO:HB2	1:31:A:ALA:H	7	0.12
(1,334)	1:26:A:PRO:HB3	1:31:A:ALA:H	7	0.12
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	16	0.12
(1,306)	1:108:A:TYR:HE1	1:112:A:GLN:HA	8	0.12
(1,306)	1:108:A:TYR:HE2	1:112:A:GLN:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB2	9	0.12
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB3	9	0.12
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB2	9	0.12
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB3	9	0.12
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	3	0.12
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	3	0.12
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	3	0.12
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB2	2	0.12
(1,283)	1:42:A:VAL:HG21	1:144:A:ASN:HB3	2	0.12
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB2	2	0.12
(1,283)	1:42:A:VAL:HG22	1:144:A:ASN:HB3	2	0.12
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB2	2	0.12
(1,283)	1:42:A:VAL:HG23	1:144:A:ASN:HB3	2	0.12
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	11	0.12
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	11	0.12
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	11	0.12
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	8	0.12
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	8	0.12
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	8	0.12
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	20	0.12
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	20	0.12
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	20	0.12
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG21	16	0.12
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG22	16	0.12
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG23	16	0.12
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	4	0.12
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	4	0.12
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	4	0.12
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	4	0.12
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	4	0.12
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	4	0.12
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	9	0.12
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	9	0.12
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	9	0.12
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	9	0.12
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	9	0.12
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	9	0.12
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD21	19	0.12
(1,249)	1:77:A:ALA:HB1	1:74:A:ASN:HD22	19	0.12
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD21	19	0.12
(1,249)	1:77:A:ALA:HB2	1:74:A:ASN:HD22	19	0.12
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD21	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:77:A:ALA:HB3	1:74:A:ASN:HD22	19	0.12
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	13	0.12
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	13	0.12
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	13	0.12
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	14	0.12
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	14	0.12
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	1	0.12
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	1	0.12
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	1	0.12
(1,198)	1:124:A:GLN:HG2	1:131:A:GLY:H	11	0.12
(1,198)	1:124:A:GLN:HG3	1:131:A:GLY:H	11	0.12
(1,192)	1:129:A:PHE:HB2	1:128:A:LEU:HB2	10	0.12
(1,192)	1:129:A:PHE:HB2	1:128:A:LEU:HB3	10	0.12
(1,192)	1:129:A:PHE:HB3	1:128:A:LEU:HB2	10	0.12
(1,192)	1:129:A:PHE:HB3	1:128:A:LEU:HB3	10	0.12
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD1	17	0.12
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD2	17	0.12
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD1	17	0.12
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD2	17	0.12
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD1	17	0.12
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD2	17	0.12
(1,151)	1:166:A:ILE:HD11	1:161:A:GLY:H	13	0.12
(1,151)	1:166:A:ILE:HD12	1:161:A:GLY:H	13	0.12
(1,151)	1:166:A:ILE:HD13	1:161:A:GLY:H	13	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	3	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	3	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	3	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	6	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	6	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	6	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	12	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	12	0.12
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	12	0.12
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB1	2	0.12
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB2	2	0.12
(1,129)	1:137:A:ILE:HG21	1:77:A:ALA:HB3	2	0.12
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB1	2	0.12
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB2	2	0.12
(1,129)	1:137:A:ILE:HG22	1:77:A:ALA:HB3	2	0.12
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB1	2	0.12
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB2	2	0.12
(1,129)	1:137:A:ILE:HG23	1:77:A:ALA:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	8	0.12
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	8	0.12
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	8	0.12
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD1	16	0.12
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD2	16	0.12
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD1	16	0.12
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD2	16	0.12
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD1	16	0.12
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD2	16	0.12
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE1	4	0.12
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE2	4	0.12
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE1	4	0.12
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE2	4	0.12
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE1	4	0.12
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE2	4	0.12
(1,50)	1:150:A:LEU:HD21	1:64:A:ASP:HA	16	0.12
(1,50)	1:150:A:LEU:HD22	1:64:A:ASP:HA	16	0.12
(1,50)	1:150:A:LEU:HD23	1:64:A:ASP:HA	16	0.12
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	20	0.12
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	20	0.12
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	20	0.12
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD1	18	0.12
(1,33)	1:27:A:VAL:HG21	1:37:A:TYR:HD2	18	0.12
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD1	18	0.12
(1,33)	1:27:A:VAL:HG22	1:37:A:TYR:HD2	18	0.12
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD1	18	0.12
(1,33)	1:27:A:VAL:HG23	1:37:A:TYR:HD2	18	0.12
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD1	20	0.12
(1,32)	1:31:A:ALA:HB1	1:37:A:TYR:HD2	20	0.12
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD1	20	0.12
(1,32)	1:31:A:ALA:HB2	1:37:A:TYR:HD2	20	0.12
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD1	20	0.12
(1,32)	1:31:A:ALA:HB3	1:37:A:TYR:HD2	20	0.12
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	19	0.12
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	19	0.12
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	19	0.12
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD11	4	0.12
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD12	4	0.12
(1,18)	1:28:A:LEU:HD11	1:133:A:LEU:HD13	4	0.12
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD11	4	0.12
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD12	4	0.12
(1,18)	1:28:A:LEU:HD12	1:133:A:LEU:HD13	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD11	4	0.12
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD12	4	0.12
(1,18)	1:28:A:LEU:HD13	1:133:A:LEU:HD13	4	0.12
(1,13)	1:142:A:MET:HE1	1:94:A:LEU:HG	16	0.12
(1,13)	1:142:A:MET:HE2	1:94:A:LEU:HG	16	0.12
(1,13)	1:142:A:MET:HE3	1:94:A:LEU:HG	16	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD11	6	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD12	6	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD13	6	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD11	6	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD12	6	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD13	6	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD11	6	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD12	6	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD13	6	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD11	12	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD12	12	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD13	12	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD11	12	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD12	12	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD13	12	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD11	12	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD12	12	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD13	12	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD11	14	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD12	14	0.12
(1,12)	1:142:A:MET:HE1	1:94:A:LEU:HD13	14	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD11	14	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD12	14	0.12
(1,12)	1:142:A:MET:HE2	1:94:A:LEU:HD13	14	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD11	14	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD12	14	0.12
(1,12)	1:142:A:MET:HE3	1:94:A:LEU:HD13	14	0.12
(1,2258)	1:137:A:ILE:HA	1:104:A:THR:H	4	0.11
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD11	2	0.11
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD12	2	0.11
(1,2246)	1:25:A:GLU:H	1:24:A:LEU:HD13	2	0.11
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG2	10	0.11
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG3	10	0.11
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG2	11	0.11
(1,2198)	1:141:A:SER:H	1:99:A:MET:HG3	11	0.11
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	7	0.11
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	11	0.11
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	14	0.11
(1,2180)	1:140:A:PHE:HD1	1:142:A:MET:H	8	0.11
(1,2180)	1:140:A:PHE:HD2	1:142:A:MET:H	8	0.11
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	1	0.11
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	6	0.11
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	9	0.11
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	12	0.11
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	2	0.11
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	2	0.11
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	2	0.11
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB2	16	0.11
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB3	16	0.11
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE1	1	0.11
(1,2091)	1:71:A:ALA:H	1:117:A:PHE:HE2	1	0.11
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG21	5	0.11
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG22	5	0.11
(1,2083)	1:61:A:CYS:H	1:45:A:VAL:HG23	5	0.11
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	2	0.11
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	2	0.11
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	13	0.11
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	13	0.11
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE1	17	0.11
(1,2082)	1:79:A:ALA:H	1:75:A:TYR:HE2	17	0.11
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD1	13	0.11
(1,2080)	1:61:A:CYS:H	1:117:A:PHE:HD2	13	0.11
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG11	16	0.11
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG12	16	0.11
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG13	16	0.11
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG11	18	0.11
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG12	18	0.11
(1,2044)	1:46:A:LEU:H	1:45:A:VAL:HG13	18	0.11
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	11	0.11
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	20	0.11
(1,2004)	1:78:A:ILE:H	1:140:A:PHE:HE1	13	0.11
(1,2004)	1:78:A:ILE:H	1:140:A:PHE:HE2	13	0.11
(1,1999)	1:149:A:ILE:HD11	1:149:A:ILE:H	8	0.11
(1,1999)	1:149:A:ILE:HD12	1:149:A:ILE:H	8	0.11
(1,1999)	1:149:A:ILE:HD13	1:149:A:ILE:H	8	0.11
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD1	1	0.11
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD1	5	0.11
(1,1981)	1:66:A:ASN:H	1:67:A:TYR:HD2	5	0.11
(1,1958)	1:16:A:ALA:H	1:14:A:VAL:HG11	11	0.11
(1,1958)	1:16:A:ALA:H	1:14:A:VAL:HG12	11	0.11
(1,1958)	1:16:A:ALA:H	1:14:A:VAL:HG13	11	0.11
(1,1954)	1:16:A:ALA:H	1:15:A:THR:HG21	11	0.11
(1,1954)	1:16:A:ALA:H	1:15:A:THR:HG22	11	0.11
(1,1954)	1:16:A:ALA:H	1:15:A:THR:HG23	11	0.11
(1,1924)	1:13:A:ARG:H	1:13:A:ARG:HG2	2	0.11
(1,1924)	1:13:A:ARG:H	1:13:A:ARG:HG3	2	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG21	5	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG22	5	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG23	5	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG21	14	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG22	14	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG23	14	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG21	18	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG22	18	0.11
(1,1922)	1:13:A:ARG:H	1:12:A:VAL:HG23	18	0.11
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	6	0.11
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	6	0.11
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	12	0.11
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	12	0.11
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD1	14	0.11
(1,1895)	1:76:A:LYS:H	1:75:A:TYR:HD2	14	0.11
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB1	13	0.11
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB2	13	0.11
(1,1862)	1:15:A:THR:H	1:16:A:ALA:HB3	13	0.11
(1,1854)	1:146:A:ASP:H	1:147:A:GLN:H	7	0.11
(1,1854)	1:146:A:ASP:H	1:147:A:GLN:H	10	0.11
(1,1854)	1:146:A:ASP:H	1:147:A:GLN:H	19	0.11
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD11	10	0.11
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD12	10	0.11
(1,1849)	1:96:A:SER:H	1:98:A:ILE:HD13	10	0.11
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG2	3	0.11
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG3	3	0.11
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG2	8	0.11
(1,1827)	1:10:A:ASP:H	1:9:A:ARG:HG3	8	0.11
(1,1808)	1:129:A:PHE:H	1:128:A:LEU:HB2	2	0.11
(1,1808)	1:129:A:PHE:H	1:128:A:LEU:HB3	2	0.11
(1,1801)	1:41:A:LYS:HD2	1:42:A:VAL:H	16	0.11
(1,1801)	1:41:A:LYS:HD3	1:42:A:VAL:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB2	7	0.11
(1,1781)	1:125:A:LYS:H	1:124:A:GLN:HB3	7	0.11
(1,1764)	1:123:A:LYS:H	1:121:A:LYS:HB2	18	0.11
(1,1764)	1:123:A:LYS:H	1:121:A:LYS:HB3	18	0.11
(1,1759)	1:54:A:THR:HB	1:55:A:LEU:H	10	0.11
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD11	9	0.11
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD12	9	0.11
(1,1733)	1:29:A:CYS:H	1:28:A:LEU:HD13	9	0.11
(1,1729)	1:171:A:GLU:H	1:170:A:ILE:HG12	17	0.11
(1,1729)	1:171:A:GLU:H	1:170:A:ILE:HG13	17	0.11
(1,1721)	1:135:A:LEU:H	1:135:A:LEU:HG	17	0.11
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB2	5	0.11
(1,1715)	1:41:A:LYS:H	1:99:A:MET:HB3	5	0.11
(1,1705)	1:47:A:ARG:H	1:61:A:CYS:H	8	0.11
(1,1689)	1:170:A:ILE:HG21	1:172:A:GLN:H	10	0.11
(1,1689)	1:170:A:ILE:HG22	1:172:A:GLN:H	10	0.11
(1,1689)	1:170:A:ILE:HG23	1:172:A:GLN:H	10	0.11
(1,1686)	1:170:A:ILE:H	1:169:A:PHE:HD1	2	0.11
(1,1686)	1:170:A:ILE:H	1:169:A:PHE:HD2	2	0.11
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB1	1	0.11
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB2	1	0.11
(1,1653)	1:84:A:LYS:H	1:80:A:ALA:HB3	1	0.11
(1,1637)	1:155:A:THR:H	1:156:A:ILE:HG13	15	0.11
(1,1596)	1:102:A:SER:H	1:101:A:HIS:HD2	13	0.11
(1,1590)	1:139:A:ASP:H	1:140:A:PHE:HA	11	0.11
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	1	0.11
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	2	0.11
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	6	0.11
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	11	0.11
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	12	0.11
(1,1557)	1:74:A:ASN:H	1:75:A:TYR:H	14	0.11
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	2	0.11
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	7	0.11
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	11	0.11
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	13	0.11
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	20	0.11
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	13	0.11
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	16	0.11
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	18	0.11
(1,1537)	1:93:A:LEU:H	1:90:A:THR:HA	20	0.11
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD21	14	0.11
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD22	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1535)	1:93:A:LEU:H	1:93:A:LEU:HD23	14	0.11
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD11	18	0.11
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD12	18	0.11
(1,1534)	1:93:A:LEU:H	1:93:A:LEU:HD13	18	0.11
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG21	11	0.11
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG22	11	0.11
(1,1474)	1:124:A:GLN:HE22	1:170:A:ILE:HG23	11	0.11
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG2	10	0.11
(1,1428)	1:171:A:GLU:HA	1:171:A:GLU:HG3	10	0.11
(1,1422)	1:170:A:ILE:HG21	1:171:A:GLU:H	15	0.11
(1,1422)	1:170:A:ILE:HG22	1:171:A:GLU:H	15	0.11
(1,1422)	1:170:A:ILE:HG23	1:171:A:GLU:H	15	0.11
(1,1357)	1:162:A:THR:HG21	1:161:A:GLY:H	1	0.11
(1,1357)	1:162:A:THR:HG22	1:161:A:GLY:H	1	0.11
(1,1357)	1:162:A:THR:HG23	1:161:A:GLY:H	1	0.11
(1,1310)	1:156:A:ILE:HB	1:157:A:GLU:H	15	0.11
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	18	0.11
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG21	15	0.11
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG22	15	0.11
(1,1294)	1:151:A:SER:HB2	1:149:A:ILE:HG23	15	0.11
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG21	15	0.11
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG22	15	0.11
(1,1294)	1:151:A:SER:HB3	1:149:A:ILE:HG23	15	0.11
(1,1266)	1:142:A:MET:HE1	1:97:A:GLU:H	6	0.11
(1,1266)	1:142:A:MET:HE2	1:97:A:GLU:H	6	0.11
(1,1266)	1:142:A:MET:HE3	1:97:A:GLU:H	6	0.11
(1,1266)	1:142:A:MET:HE1	1:97:A:GLU:H	12	0.11
(1,1266)	1:142:A:MET:HE2	1:97:A:GLU:H	12	0.11
(1,1266)	1:142:A:MET:HE3	1:97:A:GLU:H	12	0.11
(1,1263)	1:142:A:MET:HE1	1:99:A:MET:H	19	0.11
(1,1263)	1:142:A:MET:HE2	1:99:A:MET:H	19	0.11
(1,1263)	1:142:A:MET:HE3	1:99:A:MET:H	19	0.11
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	14	0.11
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	14	0.11
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	14	0.11
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	5	0.11
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	5	0.11
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	5	0.11
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	10	0.11
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	10	0.11
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	10	0.11
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	15	0.11
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	15	0.11
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	4	0.11
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	4	0.11
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	4	0.11
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	5	0.11
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	5	0.11
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	5	0.11
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	9	0.11
(1,1151)	1:125:A:LYS:HA	1:126:A:ALA:H	14	0.11
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	9	0.11
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	9	0.11
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	9	0.11
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	9	0.11
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	9	0.11
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	9	0.11
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD11	19	0.11
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD12	19	0.11
(1,1122)	1:117:A:PHE:HE1	1:60:A:LEU:HD13	19	0.11
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD11	19	0.11
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD12	19	0.11
(1,1122)	1:117:A:PHE:HE2	1:60:A:LEU:HD13	19	0.11
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	6	0.11
(1,1096)	1:113:A:VAL:HB	1:113:A:VAL:H	12	0.11
(1,1042)	1:102:A:SER:HB2	1:139:A:ASP:H	10	0.11
(1,1042)	1:102:A:SER:HB3	1:139:A:ASP:H	10	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	2	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	2	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	2	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	3	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	3	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	3	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	6	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	6	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	6	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	12	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	12	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	12	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	19	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	19	0.11
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	19	0.11
(1,1018)	1:99:A:MET:HG2	1:100:A:ILE:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:99:A:MET:HG3	1:100:A:ILE:H	11	0.11
(1,1005)	1:98:A:ILE:HG21	1:143:A:PHE:H	17	0.11
(1,1005)	1:98:A:ILE:HG22	1:143:A:PHE:H	17	0.11
(1,1005)	1:98:A:ILE:HG23	1:143:A:PHE:H	17	0.11
(1,996)	1:98:A:ILE:HD11	1:140:A:PHE:HE1	2	0.11
(1,996)	1:98:A:ILE:HD11	1:140:A:PHE:HE2	2	0.11
(1,996)	1:98:A:ILE:HD12	1:140:A:PHE:HE1	2	0.11
(1,996)	1:98:A:ILE:HD12	1:140:A:PHE:HE2	2	0.11
(1,996)	1:98:A:ILE:HD13	1:140:A:PHE:HE1	2	0.11
(1,996)	1:98:A:ILE:HD13	1:140:A:PHE:HE2	2	0.11
(1,974)	1:45:A:VAL:HG21	1:95:A:ASN:H	7	0.11
(1,974)	1:45:A:VAL:HG22	1:95:A:ASN:H	7	0.11
(1,974)	1:45:A:VAL:HG23	1:95:A:ASN:H	7	0.11
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	5	0.11
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	5	0.11
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	5	0.11
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	6	0.11
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	6	0.11
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	6	0.11
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	12	0.11
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	12	0.11
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	12	0.11
(1,954)	1:48:A:ILE:HD11	1:90:A:THR:HB	14	0.11
(1,954)	1:48:A:ILE:HD12	1:90:A:THR:HB	14	0.11
(1,954)	1:48:A:ILE:HD13	1:90:A:THR:HB	14	0.11
(1,951)	1:89:A:VAL:HG21	1:140:A:PHE:HZ	15	0.11
(1,951)	1:89:A:VAL:HG22	1:140:A:PHE:HZ	15	0.11
(1,951)	1:89:A:VAL:HG23	1:140:A:PHE:HZ	15	0.11
(1,922)	1:83:A:ARG:HA	1:83:A:ARG:HD2	9	0.11
(1,922)	1:83:A:ARG:HA	1:83:A:ARG:HD3	9	0.11
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD2	17	0.11
(1,914)	1:80:A:ALA:HB1	1:83:A:ARG:HD3	17	0.11
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD2	17	0.11
(1,914)	1:80:A:ALA:HB2	1:83:A:ARG:HD3	17	0.11
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD2	17	0.11
(1,914)	1:80:A:ALA:HB3	1:83:A:ARG:HD3	17	0.11
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	13	0.11
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	13	0.11
(1,851)	1:73:A:ALA:HB1	1:137:A:ILE:HD11	3	0.11
(1,851)	1:73:A:ALA:HB1	1:137:A:ILE:HD12	3	0.11
(1,851)	1:73:A:ALA:HB1	1:137:A:ILE:HD13	3	0.11
(1,851)	1:73:A:ALA:HB2	1:137:A:ILE:HD11	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:73:A:ALA:HB2	1:137:A:ILE:HD12	3	0.11
(1,851)	1:73:A:ALA:HB2	1:137:A:ILE:HD13	3	0.11
(1,851)	1:73:A:ALA:HB3	1:137:A:ILE:HD11	3	0.11
(1,851)	1:73:A:ALA:HB3	1:137:A:ILE:HD12	3	0.11
(1,851)	1:73:A:ALA:HB3	1:137:A:ILE:HD13	3	0.11
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD21	14	0.11
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD22	14	0.11
(1,808)	1:69:A:ILE:HG21	1:135:A:LEU:HD23	14	0.11
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD21	14	0.11
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD22	14	0.11
(1,808)	1:69:A:ILE:HG22	1:135:A:LEU:HD23	14	0.11
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD21	14	0.11
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD22	14	0.11
(1,808)	1:69:A:ILE:HG23	1:135:A:LEU:HD23	14	0.11
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	1	0.11
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	10	0.11
(1,750)	1:62:A:LEU:HA	1:62:A:LEU:HG	11	0.11
(1,748)	1:62:A:LEU:HD11	1:45:A:VAL:HA	11	0.11
(1,748)	1:62:A:LEU:HD12	1:45:A:VAL:HA	11	0.11
(1,748)	1:62:A:LEU:HD13	1:45:A:VAL:HA	11	0.11
(1,748)	1:62:A:LEU:HD11	1:45:A:VAL:HA	20	0.11
(1,748)	1:62:A:LEU:HD12	1:45:A:VAL:HA	20	0.11
(1,748)	1:62:A:LEU:HD13	1:45:A:VAL:HA	20	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	2	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	2	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	2	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	2	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	2	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	2	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	2	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	2	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	2	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	6	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	6	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	6	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	6	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	6	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	6	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	6	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	6	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	6	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	10	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	10	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	10	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	10	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	10	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	10	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	10	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	10	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	12	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	12	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	12	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	12	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	12	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	12	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	12	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	12	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	12	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	19	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	19	0.11
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	19	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	19	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	19	0.11
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	19	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	19	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	19	0.11
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	19	0.11
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD21	17	0.11
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD22	17	0.11
(1,697)	1:54:A:THR:HG21	1:55:A:LEU:HD23	17	0.11
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD21	17	0.11
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD22	17	0.11
(1,697)	1:54:A:THR:HG22	1:55:A:LEU:HD23	17	0.11
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD21	17	0.11
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD22	17	0.11
(1,697)	1:54:A:THR:HG23	1:55:A:LEU:HD23	17	0.11
(1,679)	1:48:A:ILE:HD11	1:48:A:ILE:HA	1	0.11
(1,679)	1:48:A:ILE:HD12	1:48:A:ILE:HA	1	0.11
(1,679)	1:48:A:ILE:HD13	1:48:A:ILE:HA	1	0.11
(1,676)	1:48:A:ILE:HB	1:48:A:ILE:H	8	0.11
(1,669)	1:47:A:ARG:HD2	1:48:A:ILE:H	3	0.11
(1,669)	1:47:A:ARG:HD3	1:48:A:ILE:H	3	0.11
(1,669)	1:47:A:ARG:HD2	1:48:A:ILE:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:47:A:ARG:HD3	1:48:A:ILE:H	7	0.11
(1,655)	1:42:A:VAL:HG21	1:100:A:ILE:H	5	0.11
(1,655)	1:42:A:VAL:HG22	1:100:A:ILE:H	5	0.11
(1,655)	1:42:A:VAL:HG23	1:100:A:ILE:H	5	0.11
(1,637)	1:42:A:VAL:HG21	1:99:A:MET:HA	4	0.11
(1,637)	1:42:A:VAL:HG22	1:99:A:MET:HA	4	0.11
(1,637)	1:42:A:VAL:HG23	1:99:A:MET:HA	4	0.11
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	1	0.11
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	1	0.11
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	1	0.11
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	6	0.11
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	6	0.11
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	6	0.11
(1,574)	1:33:A:LEU:HD11	1:34:A:GLY:H	12	0.11
(1,574)	1:33:A:LEU:HD12	1:34:A:GLY:H	12	0.11
(1,574)	1:33:A:LEU:HD13	1:34:A:GLY:H	12	0.11
(1,538)	1:27:A:VAL:HG11	1:26:A:PRO:HD2	17	0.11
(1,538)	1:27:A:VAL:HG12	1:26:A:PRO:HD2	17	0.11
(1,538)	1:27:A:VAL:HG13	1:26:A:PRO:HD2	17	0.11
(1,499)	1:20:A:MET:HE1	1:65:A:ALA:HA	14	0.11
(1,499)	1:20:A:MET:HE2	1:65:A:ALA:HA	14	0.11
(1,499)	1:20:A:MET:HE3	1:65:A:ALA:HA	14	0.11
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD1	1	0.11
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD2	1	0.11
(1,458)	1:55:A:LEU:HD11	1:56:A:SER:H	3	0.11
(1,458)	1:55:A:LEU:HD12	1:56:A:SER:H	3	0.11
(1,458)	1:55:A:LEU:HD13	1:56:A:SER:H	3	0.11
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	2	0.11
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	2	0.11
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	2	0.11
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	2	0.11
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	2	0.11
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	2	0.11
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	6	0.11
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	6	0.11
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	6	0.11
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	6	0.11
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	6	0.11
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	6	0.11
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	12	0.11
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	12	0.11
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	12	0.11
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	12	0.11
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	12	0.11
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG12	4	0.11
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG13	4	0.11
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG12	4	0.11
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG13	4	0.11
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG12	7	0.11
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG13	7	0.11
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG12	7	0.11
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG13	7	0.11
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG12	13	0.11
(1,432)	1:161:A:GLY:HA2	1:166:A:ILE:HG13	13	0.11
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG12	13	0.11
(1,432)	1:161:A:GLY:HA3	1:166:A:ILE:HG13	13	0.11
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG21	3	0.11
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG22	3	0.11
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG23	3	0.11
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG21	3	0.11
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG22	3	0.11
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG23	3	0.11
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG21	17	0.11
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG22	17	0.11
(1,430)	1:33:A:LEU:HB2	1:39:A:VAL:HG23	17	0.11
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG21	17	0.11
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG22	17	0.11
(1,430)	1:33:A:LEU:HB3	1:39:A:VAL:HG23	17	0.11
(1,412)	1:137:A:ILE:HD11	1:71:A:ALA:H	14	0.11
(1,412)	1:137:A:ILE:HD12	1:71:A:ALA:H	14	0.11
(1,412)	1:137:A:ILE:HD13	1:71:A:ALA:H	14	0.11
(1,412)	1:137:A:ILE:HD11	1:71:A:ALA:H	17	0.11
(1,412)	1:137:A:ILE:HD12	1:71:A:ALA:H	17	0.11
(1,412)	1:137:A:ILE:HD13	1:71:A:ALA:H	17	0.11
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	13	0.11
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	13	0.11
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB2	14	0.11
(1,405)	1:149:A:ILE:HA	1:95:A:ASN:HB3	14	0.11
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB1	5	0.11
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB2	5	0.11
(1,387)	1:84:A:LYS:HD2	1:80:A:ALA:HB3	5	0.11
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB1	5	0.11
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:84:A:LYS:HD3	1:80:A:ALA:HB3	5	0.11
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD11	5	0.11
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD12	5	0.11
(1,382)	1:78:A:ILE:HD11	1:55:A:LEU:HD13	5	0.11
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD11	5	0.11
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD12	5	0.11
(1,382)	1:78:A:ILE:HD12	1:55:A:LEU:HD13	5	0.11
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD11	5	0.11
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD12	5	0.11
(1,382)	1:78:A:ILE:HD13	1:55:A:LEU:HD13	5	0.11
(1,380)	1:134:A:VAL:HA	1:69:A:ILE:HG12	11	0.11
(1,380)	1:134:A:VAL:HA	1:69:A:ILE:HG13	11	0.11
(1,374)	1:62:A:LEU:HD21	1:69:A:ILE:H	1	0.11
(1,374)	1:62:A:LEU:HD22	1:69:A:ILE:H	1	0.11
(1,374)	1:62:A:LEU:HD23	1:69:A:ILE:H	1	0.11
(1,374)	1:62:A:LEU:HD21	1:69:A:ILE:H	17	0.11
(1,374)	1:62:A:LEU:HD22	1:69:A:ILE:H	17	0.11
(1,374)	1:62:A:LEU:HD23	1:69:A:ILE:H	17	0.11
(1,366)	1:162:A:THR:HG21	1:157:A:GLU:HB2	20	0.11
(1,366)	1:162:A:THR:HG21	1:157:A:GLU:HB3	20	0.11
(1,366)	1:162:A:THR:HG22	1:157:A:GLU:HB2	20	0.11
(1,366)	1:162:A:THR:HG22	1:157:A:GLU:HB3	20	0.11
(1,366)	1:162:A:THR:HG23	1:157:A:GLU:HB2	20	0.11
(1,366)	1:162:A:THR:HG23	1:157:A:GLU:HB3	20	0.11
(1,364)	1:47:A:ARG:HD2	1:61:A:CYS:H	7	0.11
(1,364)	1:47:A:ARG:HD3	1:61:A:CYS:H	7	0.11
(1,364)	1:47:A:ARG:HD2	1:61:A:CYS:H	9	0.11
(1,364)	1:47:A:ARG:HD3	1:61:A:CYS:H	9	0.11
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB2	1	0.11
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB3	1	0.11
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB2	1	0.11
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB3	1	0.11
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB2	1	0.11
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB3	1	0.11
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB2	17	0.11
(1,361)	1:43:A:LEU:HD11	1:64:A:ASP:HB3	17	0.11
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB2	17	0.11
(1,361)	1:43:A:LEU:HD12	1:64:A:ASP:HB3	17	0.11
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB2	17	0.11
(1,361)	1:43:A:LEU:HD13	1:64:A:ASP:HB3	17	0.11
(1,359)	1:42:A:VAL:HB	1:20:A:MET:HA	8	0.11
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB1	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB2	11	0.11
(1,337)	1:19:A:HIS:HD2	1:18:A:ALA:HB3	11	0.11
(1,336)	1:64:A:ASP:HB2	1:43:A:LEU:HG	18	0.11
(1,336)	1:64:A:ASP:HB3	1:43:A:LEU:HG	18	0.11
(1,335)	1:20:A:MET:HG2	1:65:A:ALA:HA	17	0.11
(1,335)	1:20:A:MET:HG3	1:65:A:ALA:HA	17	0.11
(1,334)	1:26:A:PRO:HB2	1:31:A:ALA:H	9	0.11
(1,334)	1:26:A:PRO:HB3	1:31:A:ALA:H	9	0.11
(1,334)	1:26:A:PRO:HB2	1:31:A:ALA:H	17	0.11
(1,334)	1:26:A:PRO:HB3	1:31:A:ALA:H	17	0.11
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	1	0.11
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	4	0.11
(1,328)	1:56:A:SER:HA	1:91:A:GLN:HE21	15	0.11
(1,326)	1:48:A:ILE:HA	1:50:A:PRO:HD3	7	0.11
(1,306)	1:108:A:TYR:HE1	1:112:A:GLN:HA	9	0.11
(1,306)	1:108:A:TYR:HE2	1:112:A:GLN:HA	9	0.11
(1,306)	1:108:A:TYR:HE1	1:112:A:GLN:HA	13	0.11
(1,306)	1:108:A:TYR:HE2	1:112:A:GLN:HA	13	0.11
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	11	0.11
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	11	0.11
(1,305)	1:75:A:TYR:HE1	1:55:A:LEU:HA	13	0.11
(1,305)	1:75:A:TYR:HE2	1:55:A:LEU:HA	13	0.11
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB2	20	0.11
(1,304)	1:67:A:TYR:HE1	1:24:A:LEU:HB3	20	0.11
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB2	20	0.11
(1,304)	1:67:A:TYR:HE2	1:24:A:LEU:HB3	20	0.11
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG21	19	0.11
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG22	19	0.11
(1,300)	1:11:A:ALA:HB1	1:12:A:VAL:HG23	19	0.11
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG21	19	0.11
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG22	19	0.11
(1,300)	1:11:A:ALA:HB2	1:12:A:VAL:HG23	19	0.11
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG21	19	0.11
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG22	19	0.11
(1,300)	1:11:A:ALA:HB3	1:12:A:VAL:HG23	19	0.11
(1,295)	1:27:A:VAL:HG21	1:23:A:TRP:HE3	5	0.11
(1,295)	1:27:A:VAL:HG22	1:23:A:TRP:HE3	5	0.11
(1,295)	1:27:A:VAL:HG23	1:23:A:TRP:HE3	5	0.11
(1,289)	1:26:A:PRO:HB2	1:30:A:GLU:H	15	0.11
(1,289)	1:26:A:PRO:HB3	1:30:A:GLU:H	15	0.11
(1,288)	1:31:A:ALA:HB1	1:33:A:LEU:HB2	13	0.11
(1,288)	1:31:A:ALA:HB1	1:33:A:LEU:HB3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:31:A:ALA:HB2	1:33:A:LEU:HB2	13	0.11
(1,288)	1:31:A:ALA:HB2	1:33:A:LEU:HB3	13	0.11
(1,288)	1:31:A:ALA:HB3	1:33:A:LEU:HB2	13	0.11
(1,288)	1:31:A:ALA:HB3	1:33:A:LEU:HB3	13	0.11
(1,284)	1:39:A:VAL:HG21	1:40:A:ASP:HA	13	0.11
(1,284)	1:39:A:VAL:HG22	1:40:A:ASP:HA	13	0.11
(1,284)	1:39:A:VAL:HG23	1:40:A:ASP:HA	13	0.11
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG11	7	0.11
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG12	7	0.11
(1,276)	1:44:A:LYS:HA	1:45:A:VAL:HG13	7	0.11
(1,272)	1:47:A:ARG:HB2	1:117:A:PHE:HD1	4	0.11
(1,272)	1:47:A:ARG:HB2	1:117:A:PHE:HD2	4	0.11
(1,272)	1:47:A:ARG:HB3	1:117:A:PHE:HD1	4	0.11
(1,272)	1:47:A:ARG:HB3	1:117:A:PHE:HD2	4	0.11
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD1	3	0.11
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD2	3	0.11
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD1	3	0.11
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD2	3	0.11
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD1	19	0.11
(1,271)	1:47:A:ARG:HG2	1:117:A:PHE:HD2	19	0.11
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD1	19	0.11
(1,271)	1:47:A:ARG:HG3	1:117:A:PHE:HD2	19	0.11
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD21	8	0.11
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD22	8	0.11
(1,269)	1:48:A:ILE:HG21	1:58:A:LEU:HD23	8	0.11
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD21	8	0.11
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD22	8	0.11
(1,269)	1:48:A:ILE:HG22	1:58:A:LEU:HD23	8	0.11
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD21	8	0.11
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD22	8	0.11
(1,269)	1:48:A:ILE:HG23	1:58:A:LEU:HD23	8	0.11
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	4	0.11
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	4	0.11
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	4	0.11
(1,260)	1:69:A:ILE:HD11	1:62:A:LEU:H	15	0.11
(1,260)	1:69:A:ILE:HD12	1:62:A:LEU:H	15	0.11
(1,260)	1:69:A:ILE:HD13	1:62:A:LEU:H	15	0.11
(1,232)	1:92:A:ASN:HB2	1:93:A:LEU:HA	11	0.11
(1,232)	1:92:A:ASN:HB3	1:93:A:LEU:HA	11	0.11
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	16	0.11
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	16	0.11
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:99:A:MET:HE1	1:40:A:ASP:HA	19	0.11
(1,229)	1:99:A:MET:HE2	1:40:A:ASP:HA	19	0.11
(1,229)	1:99:A:MET:HE3	1:40:A:ASP:HA	19	0.11
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	3	0.11
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	3	0.11
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	3	0.11
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	5	0.11
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	5	0.11
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	5	0.11
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	10	0.11
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	10	0.11
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	10	0.11
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB2	17	0.11
(1,204)	1:120:A:LEU:HG	1:117:A:PHE:HB3	17	0.11
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	13	0.11
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	13	0.11
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	13	0.11
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE2	13	0.11
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE3	13	0.11
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE2	13	0.11
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE3	13	0.11
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE2	16	0.11
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE3	16	0.11
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE2	16	0.11
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE3	16	0.11
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD21	7	0.11
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD22	7	0.11
(1,186)	1:135:A:LEU:HD21	1:24:A:LEU:HD23	7	0.11
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD21	7	0.11
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD22	7	0.11
(1,186)	1:135:A:LEU:HD22	1:24:A:LEU:HD23	7	0.11
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD21	7	0.11
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD22	7	0.11
(1,186)	1:135:A:LEU:HD23	1:24:A:LEU:HD23	7	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD1	10	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD2	10	0.11
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD1	10	0.11
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD2	10	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD1	10	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD2	10	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD1	18	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD1	18	0.11
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD2	18	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD1	18	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD2	18	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD1	19	0.11
(1,182)	1:135:A:LEU:HD21	1:103:A:PHE:HD2	19	0.11
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD1	19	0.11
(1,182)	1:135:A:LEU:HD22	1:103:A:PHE:HD2	19	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD1	19	0.11
(1,182)	1:135:A:LEU:HD23	1:103:A:PHE:HD2	19	0.11
(1,164)	1:156:A:ILE:HD11	1:66:A:ASN:HA	5	0.11
(1,164)	1:156:A:ILE:HD12	1:66:A:ASN:HA	5	0.11
(1,164)	1:156:A:ILE:HD13	1:66:A:ASN:HA	5	0.11
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	5	0.11
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	5	0.11
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	5	0.11
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	5	0.11
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	5	0.11
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	5	0.11
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	15	0.11
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	15	0.11
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	15	0.11
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	15	0.11
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	15	0.11
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	15	0.11
(1,155)	1:162:A:THR:HG21	1:67:A:TYR:HB2	10	0.11
(1,155)	1:162:A:THR:HG21	1:67:A:TYR:HB3	10	0.11
(1,155)	1:162:A:THR:HG22	1:67:A:TYR:HB2	10	0.11
(1,155)	1:162:A:THR:HG22	1:67:A:TYR:HB3	10	0.11
(1,155)	1:162:A:THR:HG23	1:67:A:TYR:HB2	10	0.11
(1,155)	1:162:A:THR:HG23	1:67:A:TYR:HB3	10	0.11
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD21	10	0.11
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD22	10	0.11
(1,134)	1:48:A:ILE:HA	1:58:A:LEU:HD23	10	0.11
(1,130)	1:134:A:VAL:HG11	1:116:A:PHE:HE1	10	0.11
(1,130)	1:134:A:VAL:HG11	1:116:A:PHE:HE2	10	0.11
(1,130)	1:134:A:VAL:HG12	1:116:A:PHE:HE1	10	0.11
(1,130)	1:134:A:VAL:HG12	1:116:A:PHE:HE2	10	0.11
(1,130)	1:134:A:VAL:HG13	1:116:A:PHE:HE1	10	0.11
(1,130)	1:134:A:VAL:HG13	1:116:A:PHE:HE2	10	0.11
(1,122)	1:114:A:GLN:HA	1:119:A:GLY:H	1	0.11
(1,122)	1:114:A:GLN:HA	1:119:A:GLY:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:114:A:GLN:HA	1:119:A:GLY:H	17	0.11
(1,89)	1:135:A:LEU:HD11	1:23:A:TRP:HZ3	13	0.11
(1,89)	1:135:A:LEU:HD12	1:23:A:TRP:HZ3	13	0.11
(1,89)	1:135:A:LEU:HD13	1:23:A:TRP:HZ3	13	0.11
(1,89)	1:135:A:LEU:HD11	1:23:A:TRP:HZ3	19	0.11
(1,89)	1:135:A:LEU:HD12	1:23:A:TRP:HZ3	19	0.11
(1,89)	1:135:A:LEU:HD13	1:23:A:TRP:HZ3	19	0.11
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	2	0.11
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	2	0.11
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	2	0.11
(1,81)	1:170:A:ILE:HD11	1:166:A:ILE:HA	11	0.11
(1,81)	1:170:A:ILE:HD12	1:166:A:ILE:HA	11	0.11
(1,81)	1:170:A:ILE:HD13	1:166:A:ILE:HA	11	0.11
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD1	5	0.11
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD2	5	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD1	5	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD2	5	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD1	5	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD2	5	0.11
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD1	6	0.11
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD2	6	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD1	6	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD2	6	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD1	6	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD2	6	0.11
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD1	12	0.11
(1,58)	1:128:A:LEU:HD21	1:129:A:PHE:HD2	12	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD1	12	0.11
(1,58)	1:128:A:LEU:HD22	1:129:A:PHE:HD2	12	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD1	12	0.11
(1,58)	1:128:A:LEU:HD23	1:129:A:PHE:HD2	12	0.11
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE1	5	0.11
(1,57)	1:128:A:LEU:HD21	1:129:A:PHE:HE2	5	0.11
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE1	5	0.11
(1,57)	1:128:A:LEU:HD22	1:129:A:PHE:HE2	5	0.11
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE1	5	0.11
(1,57)	1:128:A:LEU:HD23	1:129:A:PHE:HE2	5	0.11
(1,56)	1:45:A:VAL:HG21	1:60:A:LEU:HB2	15	0.11
(1,56)	1:45:A:VAL:HG21	1:60:A:LEU:HB3	15	0.11
(1,56)	1:45:A:VAL:HG22	1:60:A:LEU:HB2	15	0.11
(1,56)	1:45:A:VAL:HG22	1:60:A:LEU:HB3	15	0.11
(1,56)	1:45:A:VAL:HG23	1:60:A:LEU:HB2	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:45:A:VAL:HG23	1:60:A:LEU:HB3	15	0.11
(1,50)	1:150:A:LEU:HD21	1:64:A:ASP:HA	15	0.11
(1,50)	1:150:A:LEU:HD22	1:64:A:ASP:HA	15	0.11
(1,50)	1:150:A:LEU:HD23	1:64:A:ASP:HA	15	0.11
(1,35)	1:39:A:VAL:HG11	1:103:A:PHE:HZ	1	0.11
(1,35)	1:39:A:VAL:HG12	1:103:A:PHE:HZ	1	0.11
(1,35)	1:39:A:VAL:HG13	1:103:A:PHE:HZ	1	0.11
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	8	0.11
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	8	0.11
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	8	0.11
(1,23)	1:105:A:ILE:HG12	1:133:A:LEU:HD21	16	0.11
(1,23)	1:105:A:ILE:HG12	1:133:A:LEU:HD22	16	0.11
(1,23)	1:105:A:ILE:HG12	1:133:A:LEU:HD23	16	0.11
(1,23)	1:105:A:ILE:HG13	1:133:A:LEU:HD21	16	0.11
(1,23)	1:105:A:ILE:HG13	1:133:A:LEU:HD22	16	0.11
(1,23)	1:105:A:ILE:HG13	1:133:A:LEU:HD23	16	0.11
(1,2258)	1:137:A:ILE:HA	1:104:A:THR:H	14	0.1
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB1	1	0.1
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB2	1	0.1
(1,2192)	1:82:A:GLU:H	1:79:A:ALA:HB3	1	0.1
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	6	0.1
(1,2184)	1:158:A:PHE:H	1:159:A:LEU:H	12	0.1
(1,2152)	1:136:A:GLU:H	1:135:A:LEU:HG	11	0.1
(1,2139)	1:150:A:LEU:H	1:149:A:ILE:H	20	0.1
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	3	0.1
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	3	0.1
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	3	0.1
(1,2134)	1:153:A:ALA:HB1	1:150:A:LEU:H	20	0.1
(1,2134)	1:153:A:ALA:HB2	1:150:A:LEU:H	20	0.1
(1,2134)	1:153:A:ALA:HB3	1:150:A:LEU:H	20	0.1
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB2	2	0.1
(1,2127)	1:103:A:PHE:H	1:38:A:LYS:HB3	2	0.1
(1,2116)	1:72:A:PHE:H	1:73:A:ALA:HA	16	0.1
(1,2110)	1:135:A:LEU:H	1:72:A:PHE:H	11	0.1
(1,2093)	1:71:A:ALA:H	1:60:A:LEU:HG	5	0.1
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	6	0.1
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	10	0.1
(1,2021)	1:33:A:LEU:H	1:34:A:GLY:H	12	0.1
(1,1854)	1:146:A:ASP:H	1:147:A:GLN:H	11	0.1
(1,1758)	1:54:A:THR:HG21	1:55:A:LEU:H	4	0.1
(1,1758)	1:54:A:THR:HG22	1:55:A:LEU:H	4	0.1
(1,1758)	1:54:A:THR:HG23	1:55:A:LEU:H	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	15	0.1
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	15	0.1
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD1	20	0.1
(1,1690)	1:116:A:PHE:H	1:108:A:TYR:HD2	20	0.1
(1,1596)	1:102:A:SER:H	1:101:A:HIS:HD2	16	0.1
(1,1596)	1:102:A:SER:H	1:101:A:HIS:HD2	18	0.1
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	9	0.1
(1,1555)	1:74:A:ASN:H	1:76:A:LYS:H	10	0.1
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	1	0.1
(1,1553)	1:156:A:ILE:H	1:157:A:GLU:H	8	0.1
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB2	10	0.1
(1,1414)	1:170:A:ILE:HD11	1:169:A:PHE:HB3	10	0.1
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB2	10	0.1
(1,1414)	1:170:A:ILE:HD12	1:169:A:PHE:HB3	10	0.1
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB2	10	0.1
(1,1414)	1:170:A:ILE:HD13	1:169:A:PHE:HB3	10	0.1
(1,1357)	1:162:A:THR:HG21	1:161:A:GLY:H	17	0.1
(1,1357)	1:162:A:THR:HG22	1:161:A:GLY:H	17	0.1
(1,1357)	1:162:A:THR:HG23	1:161:A:GLY:H	17	0.1
(1,1350)	1:159:A:LEU:HD21	1:160:A:TYR:HB2	15	0.1
(1,1350)	1:159:A:LEU:HD21	1:160:A:TYR:HB3	15	0.1
(1,1350)	1:159:A:LEU:HD22	1:160:A:TYR:HB2	15	0.1
(1,1350)	1:159:A:LEU:HD22	1:160:A:TYR:HB3	15	0.1
(1,1350)	1:159:A:LEU:HD23	1:160:A:TYR:HB2	15	0.1
(1,1350)	1:159:A:LEU:HD23	1:160:A:TYR:HB3	15	0.1
(1,1348)	1:159:A:LEU:HD21	1:159:A:LEU:H	9	0.1
(1,1348)	1:159:A:LEU:HD22	1:159:A:LEU:H	9	0.1
(1,1348)	1:159:A:LEU:HD23	1:159:A:LEU:H	9	0.1
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	1	0.1
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	7	0.1
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	9	0.1
(1,1303)	1:155:A:THR:HB	1:156:A:ILE:H	17	0.1
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	7	0.1
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	7	0.1
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	7	0.1
(1,1247)	1:100:A:ILE:HD11	1:140:A:PHE:HA	9	0.1
(1,1247)	1:100:A:ILE:HD12	1:140:A:PHE:HA	9	0.1
(1,1247)	1:100:A:ILE:HD13	1:140:A:PHE:HA	9	0.1
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	8	0.1
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	8	0.1
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	8	0.1
(1,1213)	1:135:A:LEU:HD21	1:136:A:GLU:H	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1213)	1:135:A:LEU:HD22	1:136:A:GLU:H	15	0.1
(1,1213)	1:135:A:LEU:HD23	1:136:A:GLU:H	15	0.1
(1,1203)	1:135:A:LEU:HD11	1:135:A:LEU:H	11	0.1
(1,1203)	1:135:A:LEU:HD12	1:135:A:LEU:H	11	0.1
(1,1203)	1:135:A:LEU:HD13	1:135:A:LEU:H	11	0.1
(1,1182)	1:133:A:LEU:HD11	1:133:A:LEU:H	14	0.1
(1,1182)	1:133:A:LEU:HD12	1:133:A:LEU:H	14	0.1
(1,1182)	1:133:A:LEU:HD13	1:133:A:LEU:H	14	0.1
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD11	20	0.1
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD12	20	0.1
(1,1180)	1:133:A:LEU:HA	1:133:A:LEU:HD13	20	0.1
(1,1159)	1:109:A:ASN:HB2	1:130:A:PRO:HA	18	0.1
(1,1159)	1:109:A:ASN:HB3	1:130:A:PRO:HA	18	0.1
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG21	9	0.1
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG22	9	0.1
(1,1104)	1:70:A:LEU:HD21	1:113:A:VAL:HG23	9	0.1
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG21	9	0.1
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG22	9	0.1
(1,1104)	1:70:A:LEU:HD22	1:113:A:VAL:HG23	9	0.1
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG21	9	0.1
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG22	9	0.1
(1,1104)	1:70:A:LEU:HD23	1:113:A:VAL:HG23	9	0.1
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG21	10	0.1
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG22	10	0.1
(1,1023)	1:100:A:ILE:HB	1:137:A:ILE:HG23	10	0.1
(1,951)	1:89:A:VAL:HG21	1:140:A:PHE:HZ	19	0.1
(1,951)	1:89:A:VAL:HG22	1:140:A:PHE:HZ	19	0.1
(1,951)	1:89:A:VAL:HG23	1:140:A:PHE:HZ	19	0.1
(1,905)	1:76:A:LYS:HA	1:79:A:ALA:HB1	10	0.1
(1,905)	1:76:A:LYS:HA	1:79:A:ALA:HB2	10	0.1
(1,905)	1:76:A:LYS:HA	1:79:A:ALA:HB3	10	0.1
(1,868)	1:75:A:TYR:HD1	1:75:A:TYR:H	2	0.1
(1,868)	1:75:A:TYR:HD2	1:75:A:TYR:H	2	0.1
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD1	2	0.1
(1,824)	1:70:A:LEU:HD21	1:122:A:PHE:HD2	2	0.1
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD1	2	0.1
(1,824)	1:70:A:LEU:HD22	1:122:A:PHE:HD2	2	0.1
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD1	2	0.1
(1,824)	1:70:A:LEU:HD23	1:122:A:PHE:HD2	2	0.1
(1,822)	1:70:A:LEU:HD21	1:113:A:VAL:HA	5	0.1
(1,822)	1:70:A:LEU:HD22	1:113:A:VAL:HA	5	0.1
(1,822)	1:70:A:LEU:HD23	1:113:A:VAL:HA	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:69:A:ILE:HG21	1:24:A:LEU:HD21	14	0.1
(1,801)	1:69:A:ILE:HG21	1:24:A:LEU:HD22	14	0.1
(1,801)	1:69:A:ILE:HG21	1:24:A:LEU:HD23	14	0.1
(1,801)	1:69:A:ILE:HG22	1:24:A:LEU:HD21	14	0.1
(1,801)	1:69:A:ILE:HG22	1:24:A:LEU:HD22	14	0.1
(1,801)	1:69:A:ILE:HG22	1:24:A:LEU:HD23	14	0.1
(1,801)	1:69:A:ILE:HG23	1:24:A:LEU:HD21	14	0.1
(1,801)	1:69:A:ILE:HG23	1:24:A:LEU:HD22	14	0.1
(1,801)	1:69:A:ILE:HG23	1:24:A:LEU:HD23	14	0.1
(1,748)	1:62:A:LEU:HD11	1:45:A:VAL:HA	2	0.1
(1,748)	1:62:A:LEU:HD12	1:45:A:VAL:HA	2	0.1
(1,748)	1:62:A:LEU:HD13	1:45:A:VAL:HA	2	0.1
(1,748)	1:62:A:LEU:HD11	1:45:A:VAL:HA	10	0.1
(1,748)	1:62:A:LEU:HD12	1:45:A:VAL:HA	10	0.1
(1,748)	1:62:A:LEU:HD13	1:45:A:VAL:HA	10	0.1
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB1	5	0.1
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB2	5	0.1
(1,726)	1:60:A:LEU:HD21	1:73:A:ALA:HB3	5	0.1
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB1	5	0.1
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB2	5	0.1
(1,726)	1:60:A:LEU:HD22	1:73:A:ALA:HB3	5	0.1
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB1	5	0.1
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB2	5	0.1
(1,726)	1:60:A:LEU:HD23	1:73:A:ALA:HB3	5	0.1
(1,704)	1:55:A:LEU:HG	1:55:A:LEU:HA	5	0.1
(1,704)	1:55:A:LEU:HG	1:55:A:LEU:HA	6	0.1
(1,704)	1:55:A:LEU:HG	1:55:A:LEU:HA	12	0.1
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG2	14	0.1
(1,689)	1:50:A:PRO:HA	1:50:A:PRO:HG3	14	0.1
(1,669)	1:47:A:ARG:HD2	1:48:A:ILE:H	17	0.1
(1,669)	1:47:A:ARG:HD3	1:48:A:ILE:H	17	0.1
(1,495)	1:20:A:MET:HE1	1:20:A:MET:HA	10	0.1
(1,495)	1:20:A:MET:HE2	1:20:A:MET:HA	10	0.1
(1,495)	1:20:A:MET:HE3	1:20:A:MET:HA	10	0.1
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD1	10	0.1
(1,464)	1:89:A:VAL:HA	1:81:A:PHE:HD2	10	0.1
(1,452)	1:73:A:ALA:HB1	1:57:A:SER:HA	1	0.1
(1,452)	1:73:A:ALA:HB2	1:57:A:SER:HA	1	0.1
(1,452)	1:73:A:ALA:HB3	1:57:A:SER:HA	1	0.1
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	8	0.1
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	8	0.1
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	8	0.1
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	8	0.1
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	8	0.1
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB2	16	0.1
(1,435)	1:98:A:ILE:HG21	1:141:A:SER:HB3	16	0.1
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB2	16	0.1
(1,435)	1:98:A:ILE:HG22	1:141:A:SER:HB3	16	0.1
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB2	16	0.1
(1,435)	1:98:A:ILE:HG23	1:141:A:SER:HB3	16	0.1
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD1	2	0.1
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD2	2	0.1
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD1	2	0.1
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD2	2	0.1
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD1	2	0.1
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD2	2	0.1
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD1	10	0.1
(1,424)	1:137:A:ILE:HD11	1:140:A:PHE:HD2	10	0.1
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD1	10	0.1
(1,424)	1:137:A:ILE:HD12	1:140:A:PHE:HD2	10	0.1
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD1	10	0.1
(1,424)	1:137:A:ILE:HD13	1:140:A:PHE:HD2	10	0.1
(1,388)	1:85:A:GLU:HA	1:87:A:ARG:H	17	0.1
(1,374)	1:62:A:LEU:HD21	1:69:A:ILE:H	8	0.1
(1,374)	1:62:A:LEU:HD22	1:69:A:ILE:H	8	0.1
(1,374)	1:62:A:LEU:HD23	1:69:A:ILE:H	8	0.1
(1,366)	1:162:A:THR:HG21	1:157:A:GLU:HB2	3	0.1
(1,366)	1:162:A:THR:HG21	1:157:A:GLU:HB3	3	0.1
(1,366)	1:162:A:THR:HG22	1:157:A:GLU:HB2	3	0.1
(1,366)	1:162:A:THR:HG22	1:157:A:GLU:HB3	3	0.1
(1,366)	1:162:A:THR:HG23	1:157:A:GLU:HB2	3	0.1
(1,366)	1:162:A:THR:HG23	1:157:A:GLU:HB3	3	0.1
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD1	13	0.1
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD2	13	0.1
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD1	13	0.1
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD2	13	0.1
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD1	19	0.1
(1,351)	1:144:A:ASN:HB2	1:143:A:PHE:HD2	19	0.1
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD1	19	0.1
(1,351)	1:144:A:ASN:HB3	1:143:A:PHE:HD2	19	0.1
(1,296)	1:27:A:VAL:HG21	1:28:A:LEU:H	10	0.1
(1,296)	1:27:A:VAL:HG22	1:28:A:LEU:H	10	0.1
(1,296)	1:27:A:VAL:HG23	1:28:A:LEU:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:27:A:VAL:HG21	1:23:A:TRP:HE3	4	0.1
(1,295)	1:27:A:VAL:HG22	1:23:A:TRP:HE3	4	0.1
(1,295)	1:27:A:VAL:HG23	1:23:A:TRP:HE3	4	0.1
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG21	8	0.1
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG22	8	0.1
(1,259)	1:69:A:ILE:HB	1:134:A:VAL:HG23	8	0.1
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	8	0.1
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	8	0.1
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	8	0.1
(1,213)	1:113:A:VAL:HG21	1:122:A:PHE:HZ	14	0.1
(1,213)	1:113:A:VAL:HG22	1:122:A:PHE:HZ	14	0.1
(1,213)	1:113:A:VAL:HG23	1:122:A:PHE:HZ	14	0.1
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	8	0.1
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	8	0.1
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	8	0.1
(1,200)	1:90:A:THR:HG21	1:91:A:GLN:H	9	0.1
(1,200)	1:90:A:THR:HG22	1:91:A:GLN:H	9	0.1
(1,200)	1:90:A:THR:HG23	1:91:A:GLN:H	9	0.1
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE2	19	0.1
(1,194)	1:125:A:LYS:HB2	1:125:A:LYS:HE3	19	0.1
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE2	19	0.1
(1,194)	1:125:A:LYS:HB3	1:125:A:LYS:HE3	19	0.1
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	2	0.1
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	2	0.1
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	2	0.1
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	2	0.1
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	2	0.1
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	2	0.1
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB2	11	0.1
(1,162)	1:156:A:ILE:HG21	1:67:A:TYR:HB3	11	0.1
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB2	11	0.1
(1,162)	1:156:A:ILE:HG22	1:67:A:TYR:HB3	11	0.1
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB2	11	0.1
(1,162)	1:156:A:ILE:HG23	1:67:A:TYR:HB3	11	0.1
(1,130)	1:134:A:VAL:HG11	1:116:A:PHE:HE1	1	0.1
(1,130)	1:134:A:VAL:HG11	1:116:A:PHE:HE2	1	0.1
(1,130)	1:134:A:VAL:HG12	1:116:A:PHE:HE1	1	0.1
(1,130)	1:134:A:VAL:HG12	1:116:A:PHE:HE2	1	0.1
(1,130)	1:134:A:VAL:HG13	1:116:A:PHE:HE1	1	0.1
(1,130)	1:134:A:VAL:HG13	1:116:A:PHE:HE2	1	0.1
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD2	19	0.1
(1,97)	1:9:A:ARG:HA	1:9:A:ARG:HD3	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:150:A:LEU:HD21	1:64:A:ASP:HA	4	0.1
(1,50)	1:150:A:LEU:HD22	1:64:A:ASP:HA	4	0.1
(1,50)	1:150:A:LEU:HD23	1:64:A:ASP:HA	4	0.1
(1,46)	1:33:A:LEU:HD11	1:103:A:PHE:HZ	1	0.1
(1,46)	1:33:A:LEU:HD12	1:103:A:PHE:HZ	1	0.1
(1,46)	1:33:A:LEU:HD13	1:103:A:PHE:HZ	1	0.1
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG21	7	0.1
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG22	7	0.1
(1,43)	1:33:A:LEU:HD21	1:39:A:VAL:HG23	7	0.1
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG21	7	0.1
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG22	7	0.1
(1,43)	1:33:A:LEU:HD22	1:39:A:VAL:HG23	7	0.1
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG21	7	0.1
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG22	7	0.1
(1,43)	1:33:A:LEU:HD23	1:39:A:VAL:HG23	7	0.1
(1,30)	1:39:A:VAL:HG11	1:23:A:TRP:HZ3	20	0.1
(1,30)	1:39:A:VAL:HG12	1:23:A:TRP:HZ3	20	0.1
(1,30)	1:39:A:VAL:HG13	1:23:A:TRP:HZ3	20	0.1
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD1	10	0.1
(1,25)	1:105:A:ILE:HG12	1:169:A:PHE:HD2	10	0.1
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD1	10	0.1
(1,25)	1:105:A:ILE:HG13	1:169:A:PHE:HD2	10	0.1
(1,13)	1:142:A:MET:HE1	1:94:A:LEU:HG	9	0.1
(1,13)	1:142:A:MET:HE2	1:94:A:LEU:HG	9	0.1
(1,13)	1:142:A:MET:HE3	1:94:A:LEU:HG	9	0.1

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

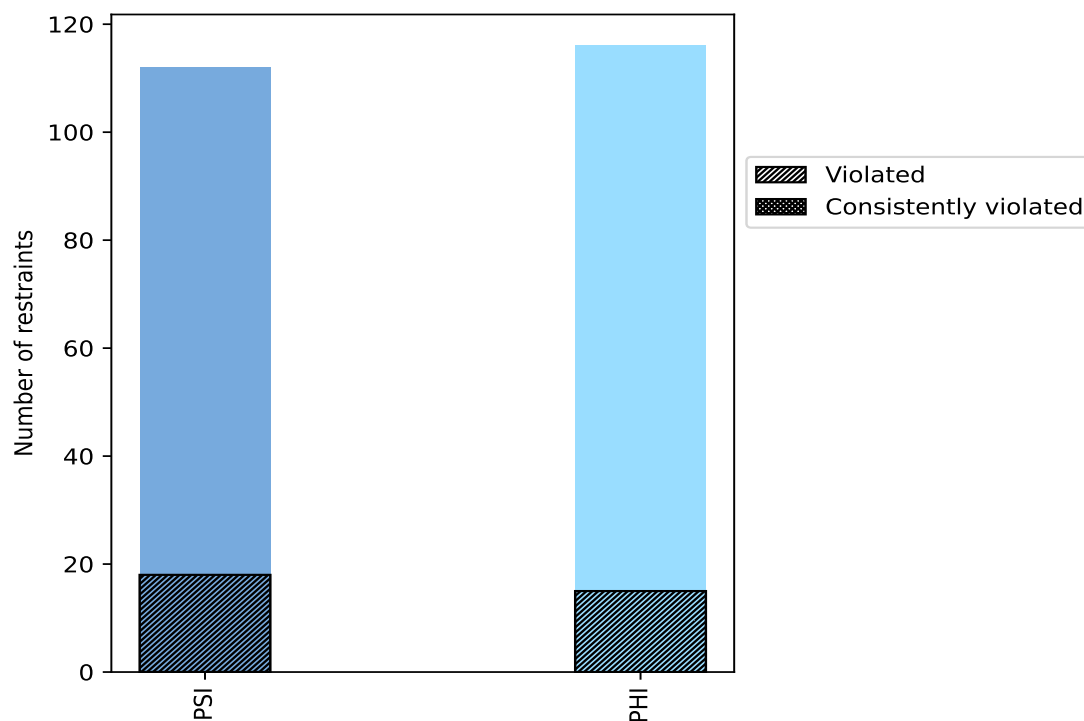
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	112	49.1	18	16.1	7.9	0	0.0	0.0
PHI	116	50.9	15	12.9	6.6	0	0.0	0.0
Total	228	100.0	33	14.5	14.5	0	0.0	0.0

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

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



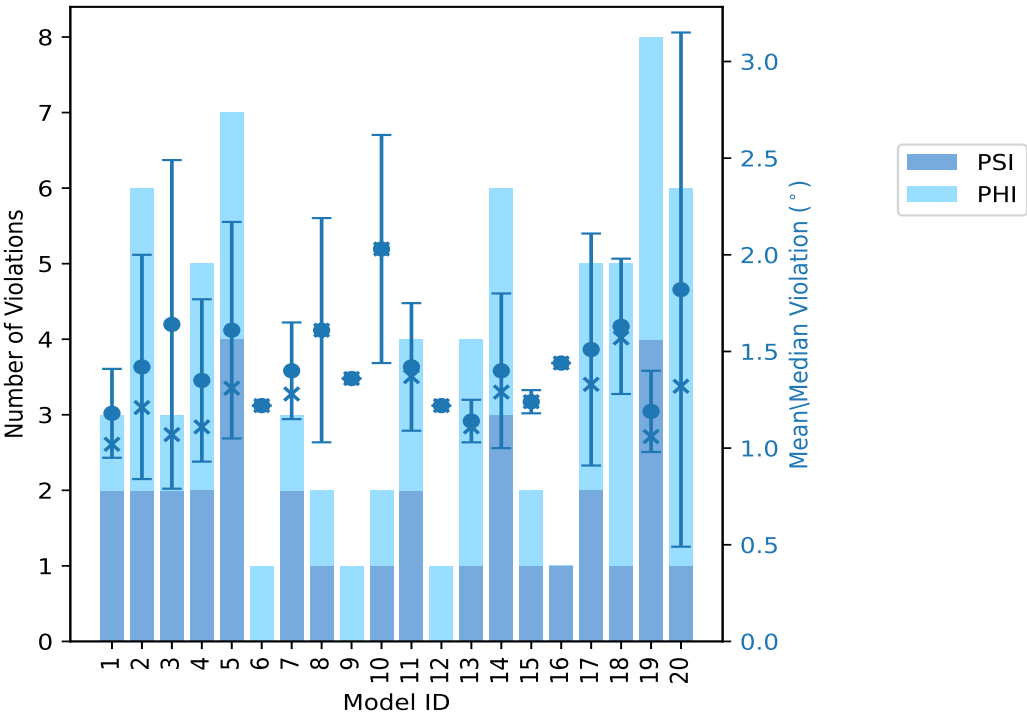
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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	2	1	3	1.18	1.51	0.23	1.02
2	2	4	6	1.42	2.66	0.58	1.21
3	2	1	3	1.64	2.84	0.85	1.07
4	2	3	5	1.35	2.16	0.42	1.11
5	4	3	7	1.61	2.45	0.56	1.31
6	0	1	1	1.22	1.22	0.0	1.22
7	2	1	3	1.4	1.75	0.25	1.28
8	1	1	2	1.61	2.19	0.58	1.61
9	0	1	1	1.36	1.36	0.0	1.36
10	1	1	2	2.03	2.62	0.59	2.03
11	2	2	4	1.42	1.85	0.33	1.37
12	0	1	1	1.22	1.22	0.0	1.22
13	1	3	4	1.14	1.31	0.11	1.11
14	3	3	6	1.4	2.06	0.4	1.29
15	1	1	2	1.24	1.3	0.06	1.24
16	1	0	1	1.44	1.44	0.0	1.44
17	2	3	5	1.51	2.69	0.6	1.33
18	1	4	5	1.63	2.22	0.35	1.57
19	4	4	8	1.19	1.5	0.21	1.06
20	1	5	6	1.82	4.78	1.33	1.32

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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 <sup>1</sup>	%
10	6	16	1	5.0
4	3	7	2	10.0
3	3	6	3	15.0
0	0	0	4	20.0
1	0	1	5	25.0
0	1	1	6	30.0
0	0	0	7	35.0
0	2	2	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

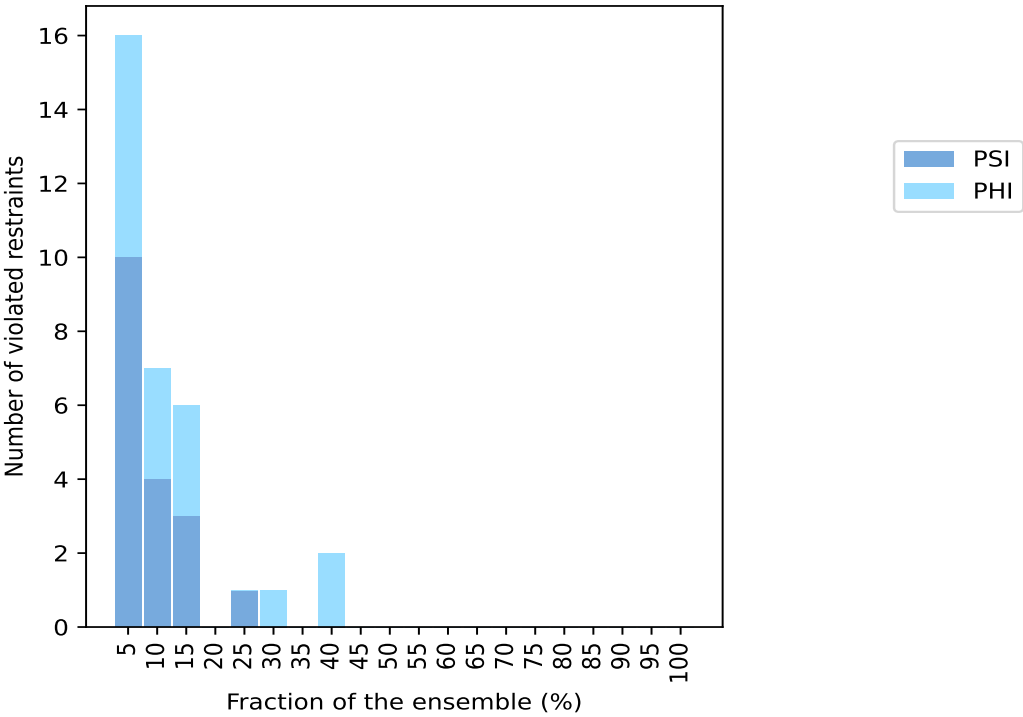
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

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

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



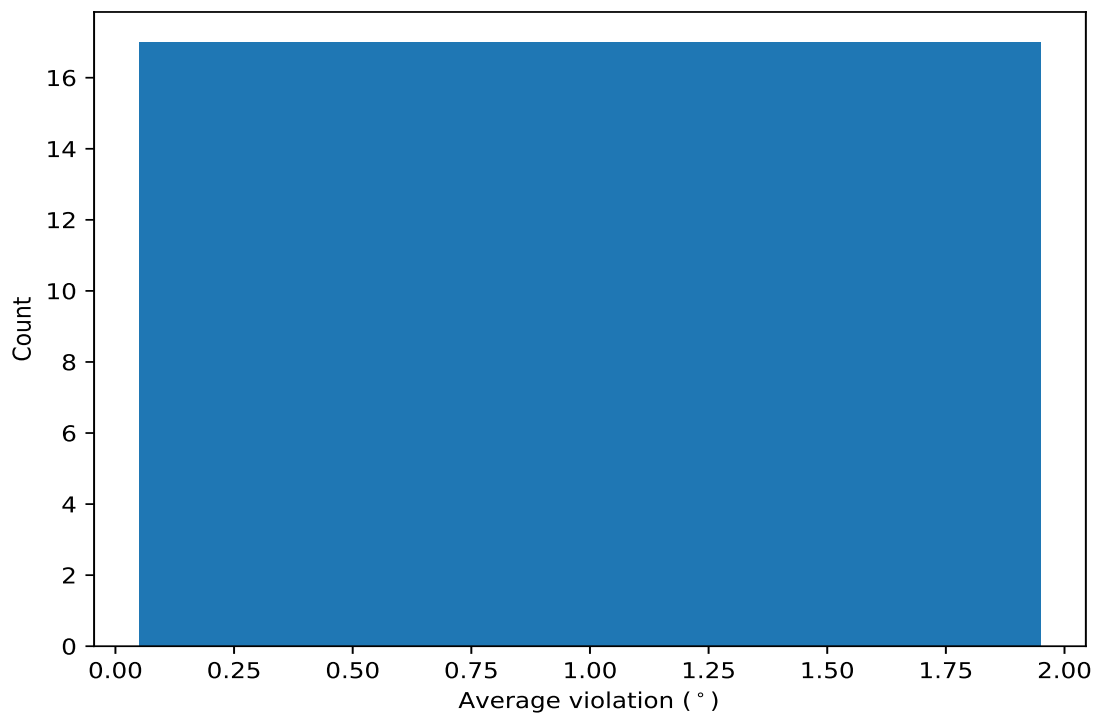
10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 [i](#)

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

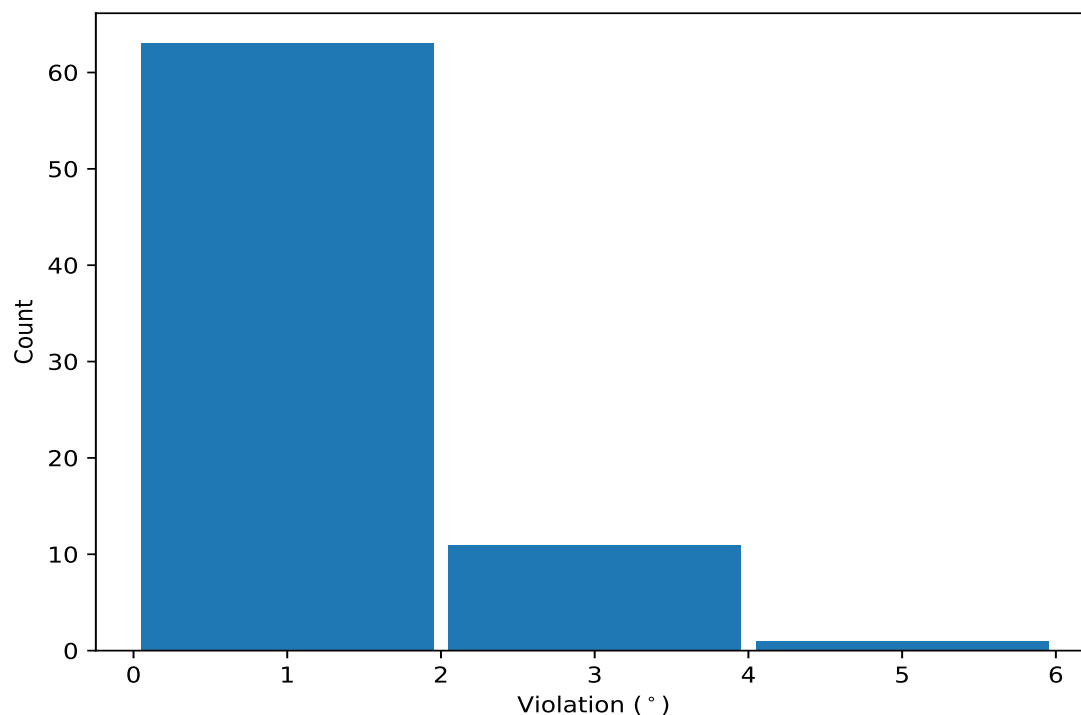
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	8	1.98	0.47	2.12
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	8	1.78	0.58	1.6
(1,21)	1:48:A:ILE:C	1:49:A:TYR:N	1:49:A:TYR:CA	1:49:A:TYR:C	6	1.53	0.54	1.32
(1,159)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:PHE:N	5	1.16	0.18	1.07
(1,168)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:GLN:N	3	1.4	0.27	1.44
(1,163)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:ARG:N	3	1.37	0.23	1.44
(1,40)	1:74:A:ASN:C	1:75:A:TYR:N	1:75:A:TYR:CA	1:75:A:TYR:C	3	1.23	0.15	1.31
(1,1)	1:22:A:HIS:C	1:23:A:TRP:N	1:23:A:TRP:CA	1:23:A:TRP:C	3	1.19	0.27	1.01
(1,42)	1:76:A:LYS:C	1:77:A:ALA:N	1:77:A:ALA:CA	1:77:A:ALA:C	3	1.09	0.05	1.11
(1,120)	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	1:28:A:LEU:N	3	1.09	0.07	1.05
(1,190)	1:119:A:GLY:N	1:119:A:GLY:CA	1:119:A:GLY:C	1:120:A:LEU:N	2	1.64	0.53	1.64
(1,5)	1:27:A:VAL:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	2	1.43	0.1	1.43
(1,47)	1:81:A:PHE:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	2	1.38	0.08	1.38
(1,135)	1:47:A:ARG:N	1:47:A:ARG:CA	1:47:A:ARG:C	1:48:A:ILE:N	2	1.25	0.2	1.25
(1,81)	1:121:A:LYS:C	1:122:A:PHE:N	1:122:A:PHE:CA	1:122:A:PHE:C	2	1.19	0.17	1.19
(1,123)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:ALA:N	2	1.12	0.06	1.12
(1,181)	1:109:A:ASN:N	1:109:A:ASN:CA	1:109:A:ASN:C	1:110:A:ASP:N	2	1.02	0.01	1.02

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,209)	1:143:A:PHE:N	1:143:A:PHE:CA	1:143:A:PHE:C	1:144:A:ASN:N	20	4.78
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	3	2.84
(1,21)	1:48:A:ILE:C	1:49:A:TYR:N	1:49:A:TYR:CA	1:49:A:TYR:C	17	2.69
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	2	2.66
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	10	2.62
(1,107)	1:158:A:PHE:C	1:159:A:LEU:N	1:159:A:LEU:CA	1:159:A:LEU:C	5	2.45
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	18	2.22
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	8	2.19
(1,190)	1:119:A:GLY:N	1:119:A:GLY:CA	1:119:A:GLY:C	1:120:A:LEU:N	5	2.17
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	4	2.16
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	5	2.08
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	14	2.06
(1,85)	1:128:A:LEU:C	1:129:A:PHE:N	1:129:A:PHE:CA	1:129:A:PHE:C	11	1.85
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	7	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,168)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:GLN:N	14	1.72
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	18	1.69
(1,163)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:ARG:N	11	1.62
(1,1)	1:22:A:HIS:C	1:23:A:TRP:N	1:23:A:TRP:CA	1:23:A:TRP:C	18	1.57
(1,5)	1:27:A:VAL:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	18	1.53
(1,21)	1:48:A:ILE:C	1:49:A:TYR:N	1:49:A:TYR:CA	1:49:A:TYR:C	14	1.52
(1,159)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:PHE:N	1	1.51
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	19	1.5
(1,47)	1:81:A:PHE:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	19	1.47
(1,135)	1:47:A:ARG:N	1:47:A:ARG:CA	1:47:A:ARG:C	1:48:A:ILE:N	2	1.45
(1,168)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:GLN:N	16	1.44
(1,163)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:ARG:N	10	1.44
(1,17)	1:44:A:LYS:C	1:45:A:VAL:N	1:45:A:VAL:CA	1:45:A:VAL:C	19	1.4
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	17	1.38
(1,81)	1:121:A:LYS:C	1:122:A:PHE:N	1:122:A:PHE:CA	1:122:A:PHE:C	2	1.36
(1,40)	1:74:A:ASN:C	1:75:A:TYR:N	1:75:A:TYR:CA	1:75:A:TYR:C	20	1.36
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	9	1.36
(1,167)	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1:90:A:THR:N	17	1.33
(1,21)	1:48:A:ILE:C	1:49:A:TYR:N	1:49:A:TYR:CA	1:49:A:TYR:C	4	1.33
(1,5)	1:27:A:VAL:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	20	1.33
(1,40)	1:74:A:ASN:C	1:75:A:TYR:N	1:75:A:TYR:CA	1:75:A:TYR:C	13	1.31
(1,21)	1:48:A:ILE:C	1:49:A:TYR:N	1:49:A:TYR:CA	1:49:A:TYR:C	5	1.31
(1,21)	1:48:A:ILE:C	1:49:A:TYR:N	1:49:A:TYR:CA	1:49:A:TYR:C	20	1.31
(1,47)	1:81:A:PHE:C	1:82:A:GLU:N	1:82:A:GLU:CA	1:82:A:GLU:C	15	1.3
(1,225)	1:168:A:ARG:N	1:168:A:ARG:CA	1:168:A:ARG:C	1:169:A:PHE:N	7	1.28
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	6	1.22
(1,2)	1:24:A:LEU:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	12	1.22
(1,219)	1:161:A:GLY:N	1:161:A:GLY:CA	1:161:A:GLY:C	1:162:A:THR:N	5	1.18
(1,123)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:ALA:N	7	1.18
(1,120)	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	1:28:A:LEU:N	15	1.18
(1,42)	1:76:A:LYS:C	1:77:A:ALA:N	1:77:A:ALA:CA	1:77:A:ALA:C	20	1.15
(1,118)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:PRO:N	18	1.14
(1,190)	1:119:A:GLY:N	1:119:A:GLY:CA	1:119:A:GLY:C	1:120:A:LEU:N	13	1.11
(1,159)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:PHE:N	4	1.11
(1,51)	1:85:A:GLU:C	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	13	1.11
(1,42)	1:76:A:LYS:C	1:77:A:ALA:N	1:77:A:ALA:CA	1:77:A:ALA:C	17	1.11
(1,3)	1:25:A:GLU:C	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	11	1.11
(1,121)	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	1:29:A:CYS:N	4	1.1
(1,140)	1:53:A:ASN:N	1:53:A:ASN:CA	1:53:A:ASN:C	1:54:A:THR:N	11	1.08
(1,159)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:PHE:N	3	1.07
(1,163)	1:85:A:GLU:N	1:85:A:GLU:CA	1:85:A:GLU:C	1:86:A:ARG:N	2	1.06
(1,159)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:PHE:N	19	1.06
(1,148)	1:67:A:TYR:N	1:67:A:TYR:CA	1:67:A:TYR:C	1:68:A:LYS:N	14	1.06
(1,168)	1:90:A:THR:N	1:90:A:THR:CA	1:90:A:THR:C	1:91:A:GLN:N	19	1.05
(1,135)	1:47:A:ARG:N	1:47:A:ARG:CA	1:47:A:ARG:C	1:48:A:ILE:N	5	1.05
(1,123)	1:30:A:GLU:N	1:30:A:GLU:CA	1:30:A:GLU:C	1:31:A:ALA:N	17	1.05
(1,120)	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	1:28:A:LEU:N	19	1.05
(1,181)	1:109:A:ASN:N	1:109:A:ASN:CA	1:109:A:ASN:C	1:110:A:ASP:N	14	1.03
(1,159)	1:80:A:ALA:N	1:80:A:ALA:CA	1:80:A:ALA:C	1:81:A:PHE:N	8	1.03
(1,120)	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	1:28:A:LEU:N	5	1.03
(1,40)	1:74:A:ASN:C	1:75:A:TYR:N	1:75:A:TYR:CA	1:75:A:TYR:C	4	1.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,122)	1:29:A:CYS:N	1:29:A:CYS:CA	1:29:A:CYS:C	1:30:A:GLU:N	1	1.02
(1,92)	1:137:A:ILE:C	1:138:A:ASN:N	1:138:A:ASN:CA	1:138:A:ASN:C	19	1.02
(1,81)	1:121:A:LYS:C	1:122:A:PHE:N	1:122:A:PHE:CA	1:122:A:PHE:C	14	1.02
(1,42)	1:76:A:LYS:C	1:77:A:ALA:N	1:77:A:ALA:CA	1:77:A:ALA:C	1	1.02
(1,181)	1:109:A:ASN:N	1:109:A:ASN:CA	1:109:A:ASN:C	1:110:A:ASP:N	3	1.01
(1,49)	1:83:A:ARG:C	1:84:A:LYS:N	1:84:A:LYS:CA	1:84:A:LYS:C	13	1.01
(1,21)	1:48:A:ILE:C	1:49:A:TYR:N	1:49:A:TYR:CA	1:49:A:TYR:C	2	1.01
(1,1)	1:22:A:HIS:C	1:23:A:TRP:N	1:23:A:TRP:CA	1:23:A:TRP:C	2	1.01
(1,124)	1:31:A:ALA:N	1:31:A:ALA:CA	1:31:A:ALA:C	1:32:A:GLY:N	19	1.0
(1,1)	1:22:A:HIS:C	1:23:A:TRP:N	1:23:A:TRP:CA	1:23:A:TRP:C	20	1.0