



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 03:57 AM EST

PDB ID : 5JTO  
BMRB ID : 30083  
Title : The structure of chaperone SecB in complex with unstructured proPhoA binding site d  
Authors : Huang, C.; Saio, T.; Rossi, P.; Kalodimos, C.G.  
Deposited on : 2016-05-09

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

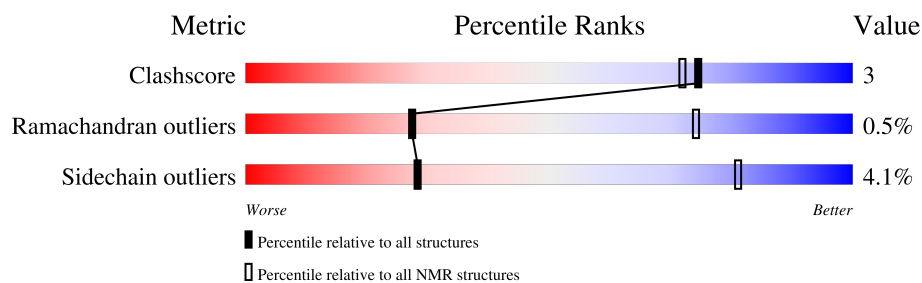
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 53%.

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	155	76% 5% 19%
1	B	155	75% 5% 20%
1	C	155	79% 19%
1	D	155	75% 5% 20%
2	E	40	100%
2	F	40	100%
2	G	40	100%
2	H	40	100%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:10-A:134, B:10-B:133, C:9-C:134, D:10-D:133 (499)	0.91	5

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11912 atoms, of which 5848 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein-export protein SecB.

Mol	Chain	Residues	Atoms						Trace
1	A	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	
1	B	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	
1	C	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	
1	D	155	Total	C	H	N	O	S	0
			2367	762	1155	198	243	9	

- Molecule 2 is a protein called Alkaline phosphatase.

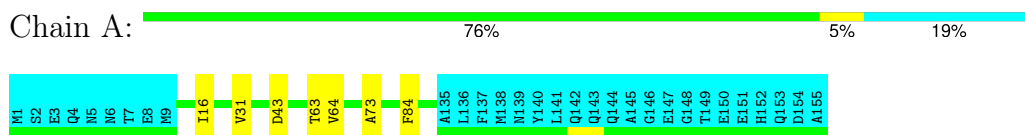
Mol	Chain	Residues	Atoms						Trace
2	E	40	Total	C	H	N	O	S	0
			611	194	307	54	54	2	
2	F	40	Total	C	H	N	O	S	0
			611	194	307	54	54	2	
2	G	40	Total	C	H	N	O	S	0
			611	194	307	54	54	2	
2	H	40	Total	C	H	N	O	S	0
			611	194	307	54	54	2	

## 4 Residue-property plots

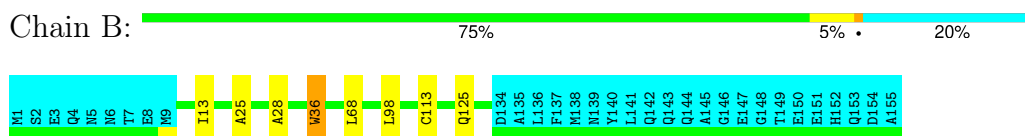
### 4.1 Average score per residue in the NMR ensemble

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.

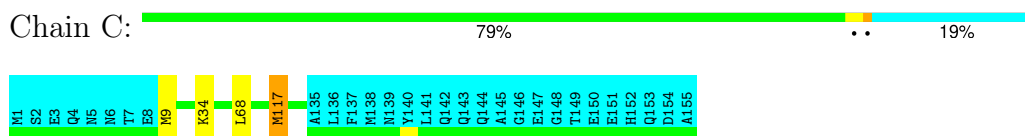
- Molecule 1: Protein-export protein SecB



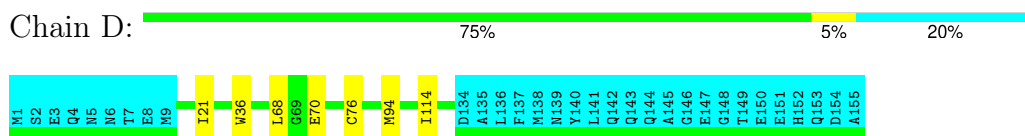
- Molecule 1: Protein-export protein SecB



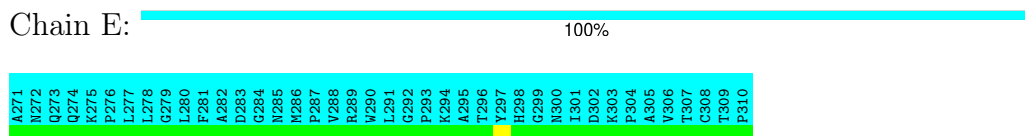
- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB

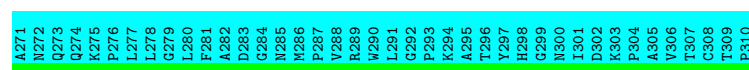


- Molecule 2: Alkaline phosphatase



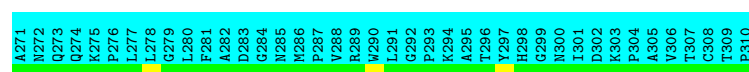
- Molecule 2: Alkaline phosphatase

Chain F:  100%



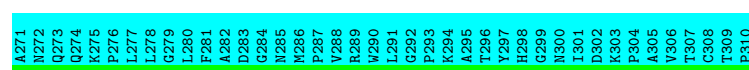
- Molecule 2: Alkaline phosphatase

Chain G:  100%



- Molecule 2: Alkaline phosphatase

Chain H:  100%



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

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

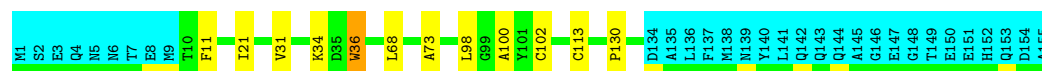
- Molecule 1: Protein-export protein SecB

Chain A:  74% 6% 19%



- Molecule 1: Protein-export protein SecB

Chain B:  72% 7% 20%

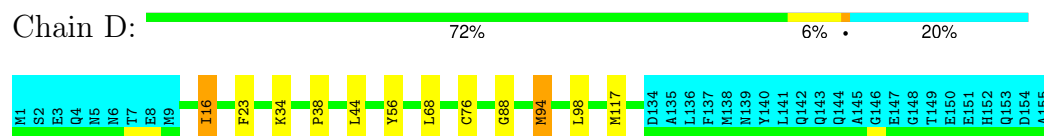


- Molecule 1: Protein-export protein SecB

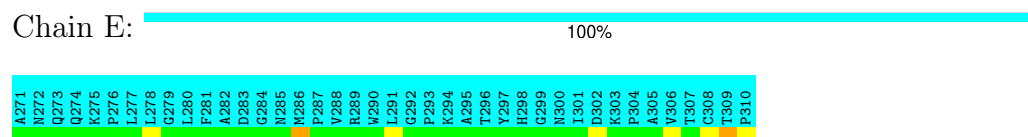
Chain C:  72% 9% 19%



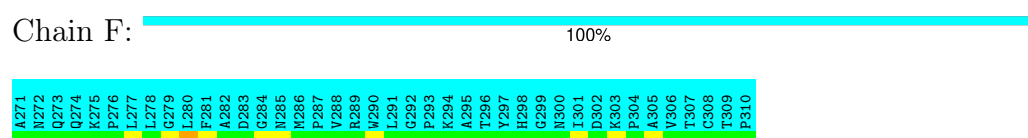
- Molecule 1: Protein-export protein SecB



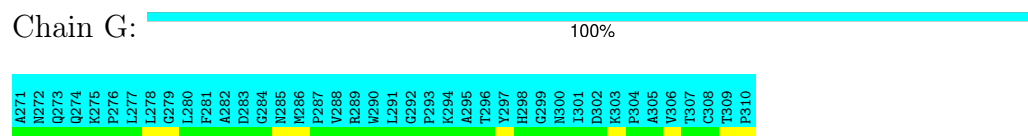
- Molecule 2: Alkaline phosphatase



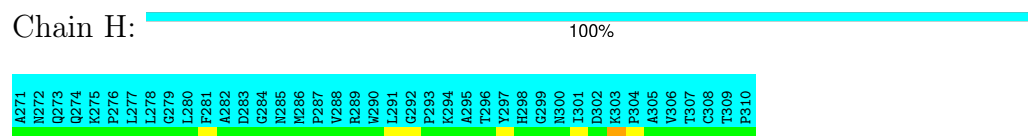
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

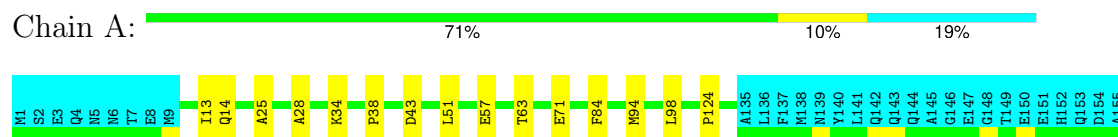


- Molecule 2: Alkaline phosphatase

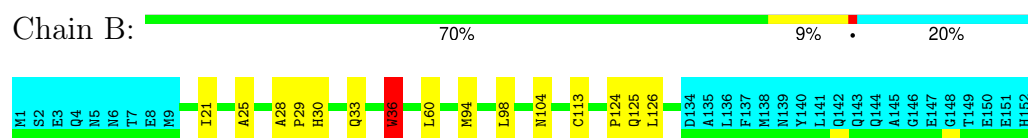


#### 4.2.2 Score per residue for model 2

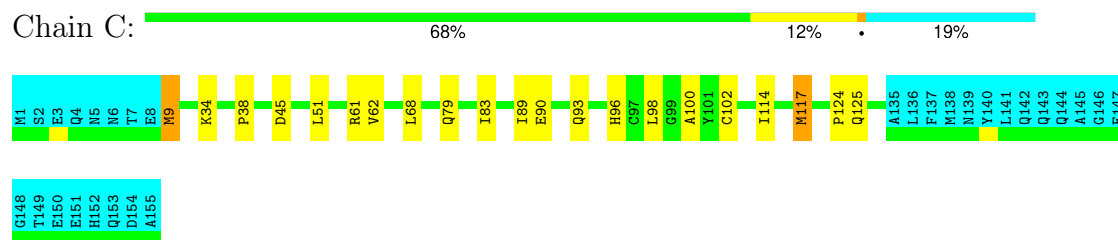
- Molecule 1: Protein-export protein SecB



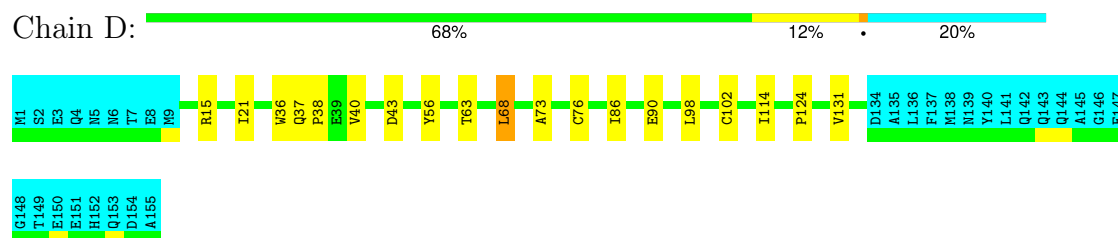
- Molecule 1: Protein-export protein SecB



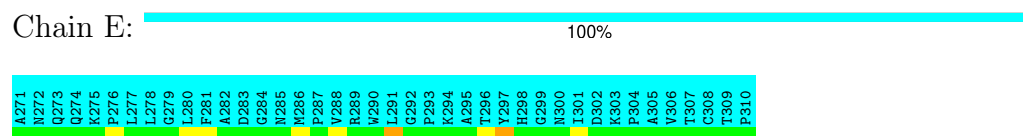
- Molecule 1: Protein-export protein SecB



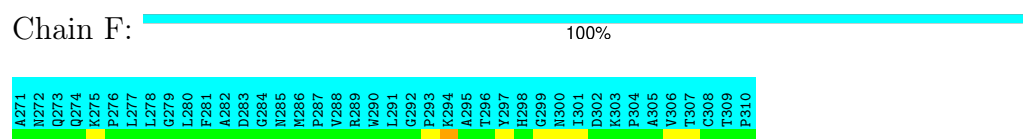
- Molecule 1: Protein-export protein SecB



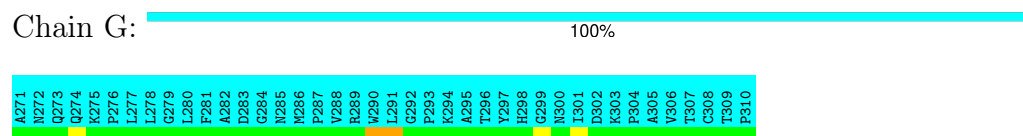
- Molecule 2: Alkaline phosphatase



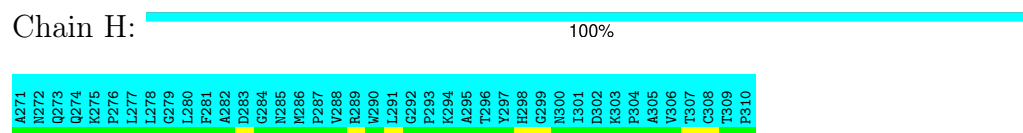
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase



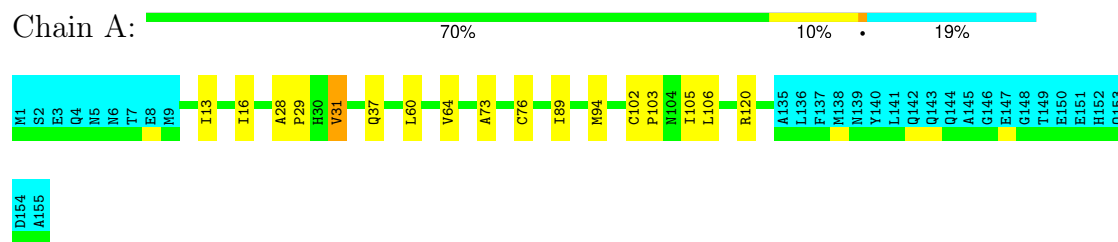
- Molecule 2: Alkaline phosphatase



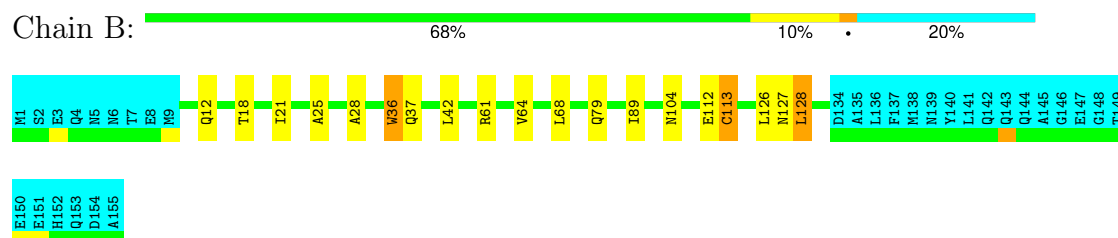
#### 4.2.3 Score per residue for model 3

- Molecule 1: Protein-export protein SecB

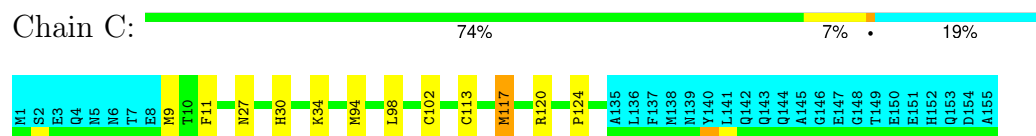




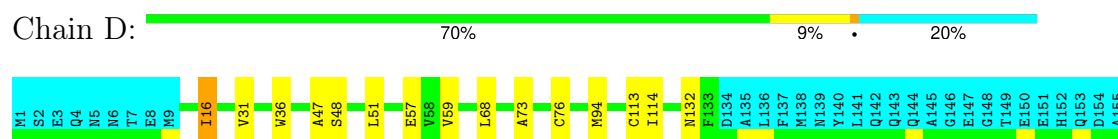
- Molecule 1: Protein-export protein SecB



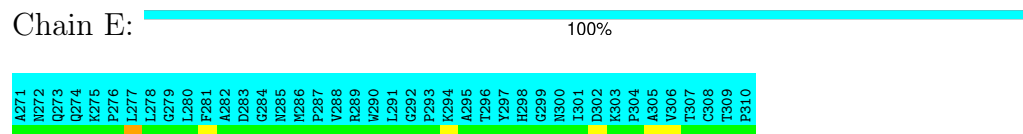
- Molecule 1: Protein-export protein SecB



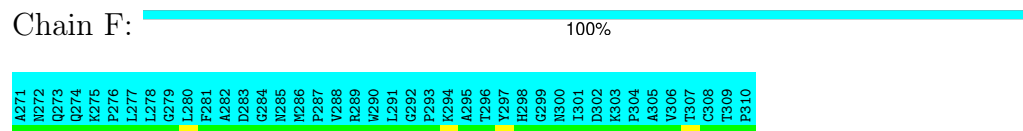
- Molecule 1: Protein-export protein SecB



- Molecule 2: Alkaline phosphatase

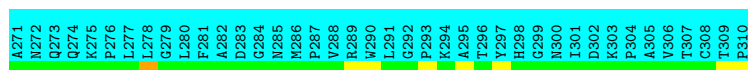


- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase





- Molecule 2: Alkaline phosphatase

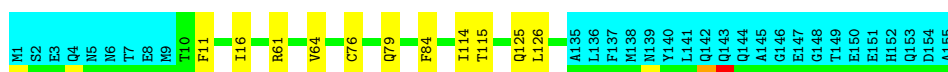
Chain H: 100%



#### 4.2.4 Score per residue for model 4

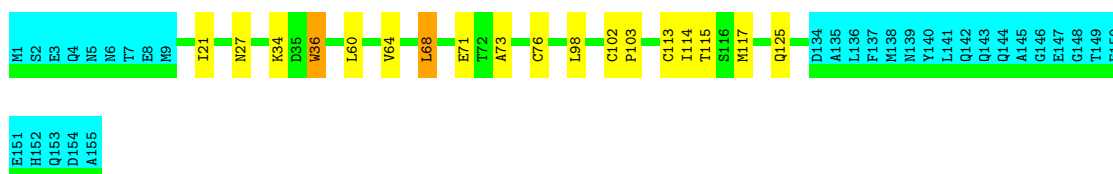
- Molecule 1: Protein-export protein SecB

Chain A: 74% 7% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 68% 10% 20%



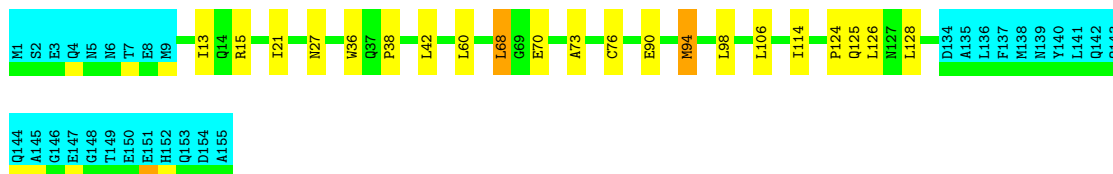
- Molecule 1: Protein-export protein SecB

Chain C: 75% 5% 19%



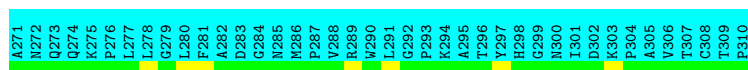
- Molecule 1: Protein-export protein SecB

Chain D: 66% 12% 20%



- Molecule 2: Alkaline phosphatase

Chain E: 100%



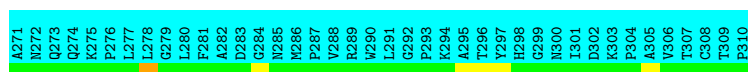
- Molecule 2: Alkaline phosphatase

Chain F: 100%



- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

Chain H: 100%



#### 4.2.5 Score per residue for model 5 (medoid)

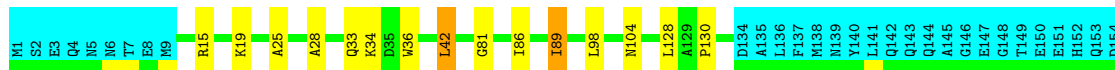
- Molecule 1: Protein-export protein SecB

Chain A: 70% 11% 19%



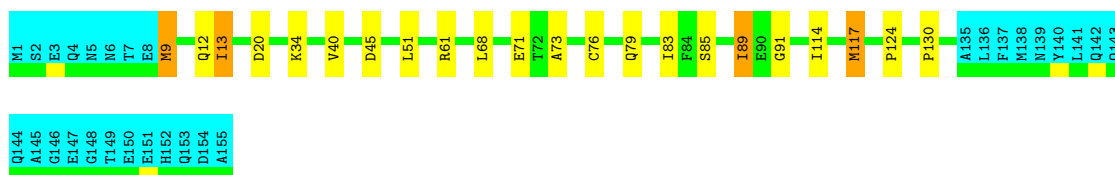
- Molecule 1: Protein-export protein SecB

Chain B: 70% 8% 20%



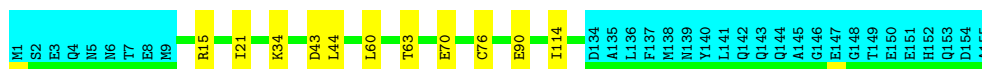
- Molecule 1: Protein-export protein SecB

Chain C: 67% 12% 19%



- Molecule 1: Protein-export protein SecB

Chain D: 73% 7% 20%



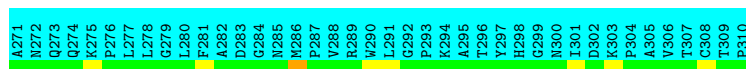
- Molecule 2: Alkaline phosphatase

Chain E: 100%



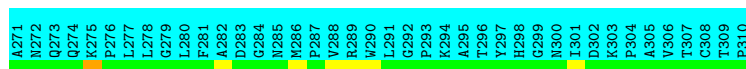
- Molecule 2: Alkaline phosphatase

Chain F: 100%



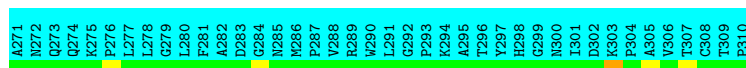
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

Chain H: 100%



#### 4.2.6 Score per residue for model 6

- Molecule 1: Protein-export protein SecB

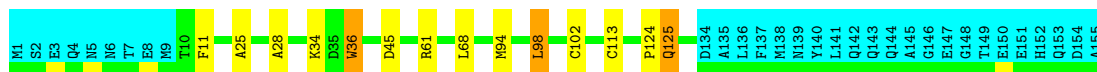
Chain A: 68% 12% 19%





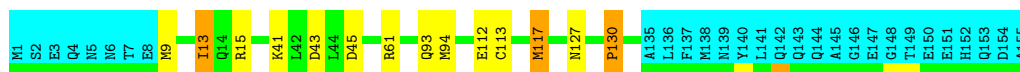
• Molecule 1: Protein-export protein SecB

Chain B: 71% 7% 20%



• Molecule 1: Protein-export protein SecB

Chain C: 72% 7% 19%



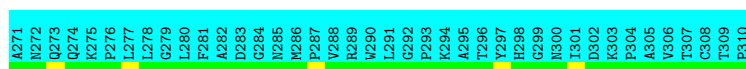
• Molecule 1: Protein-export protein SecB

Chain D: 73% 7% 20%



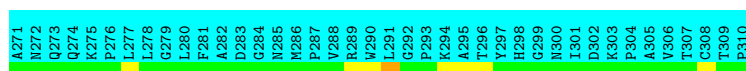
• Molecule 2: Alkaline phosphatase

Chain E: 100%



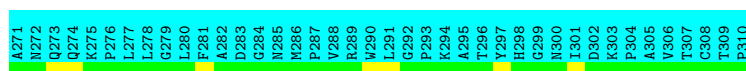
• Molecule 2: Alkaline phosphatase

Chain F: 100%



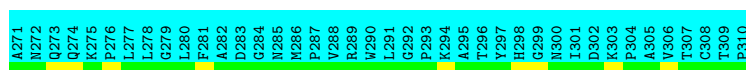
• Molecule 2: Alkaline phosphatase

Chain G: 100%



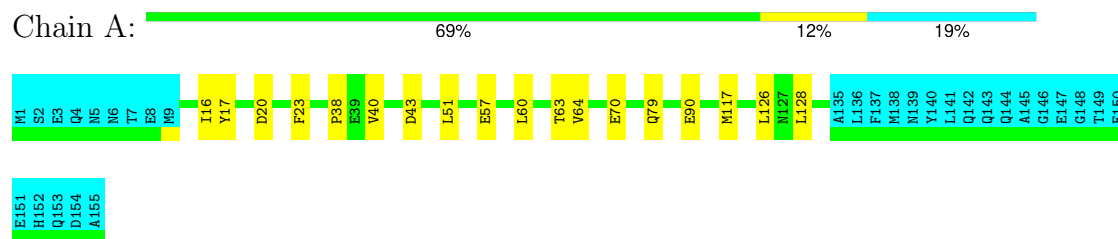
• Molecule 2: Alkaline phosphatase

Chain H: 100%

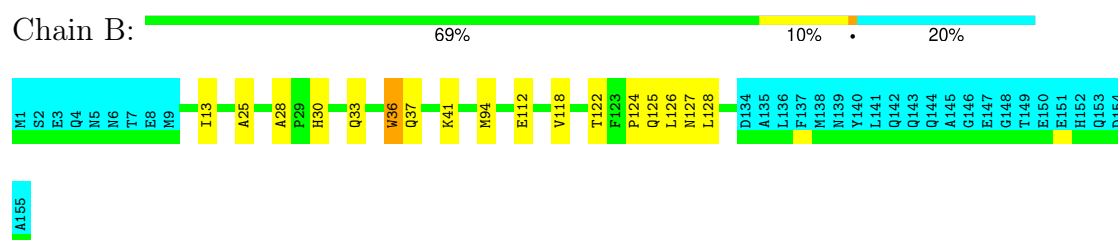


### 4.2.7 Score per residue for model 7

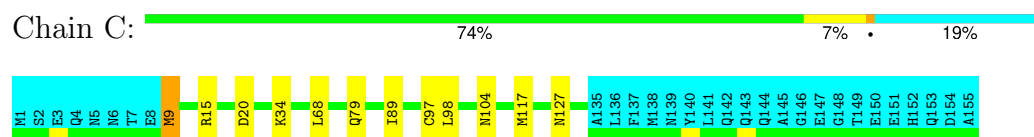
- Molecule 1: Protein-export protein SecB



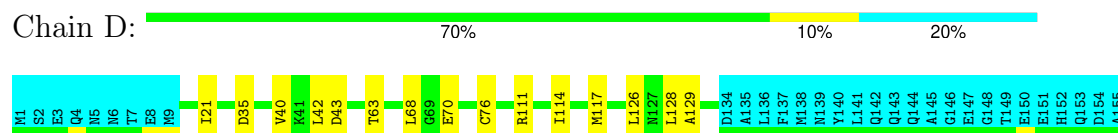
- Molecule 1: Protein-export protein SecB



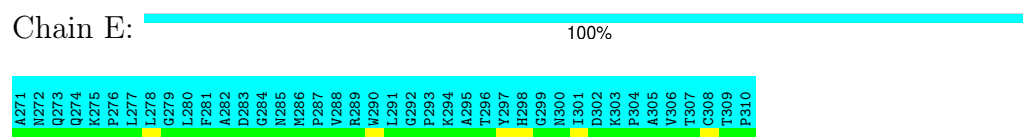
- Molecule 1: Protein-export protein SecB



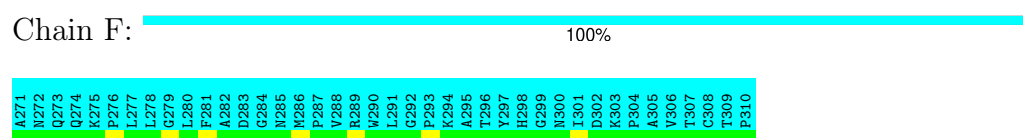
- Molecule 1: Protein-export protein SecB



- Molecule 2: Alkaline phosphatase

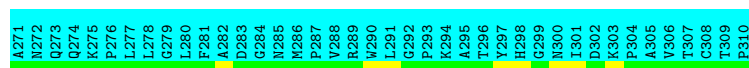


- Molecule 2: Alkaline phosphatase



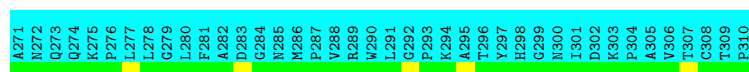
- Molecule 2: Alkaline phosphatase

Chain G:  100%



- Molecule 2: Alkaline phosphatase

Chain H:  100%



## 4.2.8 Score per residue for model 8

- Molecule 1: Protein-export protein SecB

Chain A:  72% 8% 19%



- Molecule 1: Protein-export protein SecB

Chain B:  71% 8% 20%



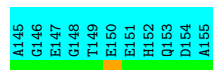
- Molecule 1: Protein-export protein SecB

Chain C:  68% 10% 19%



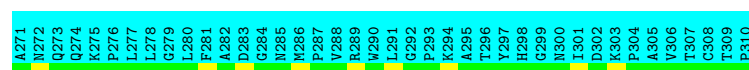
- Molecule 1: Protein-export protein SecB

Chain D:  67% 13% 20%



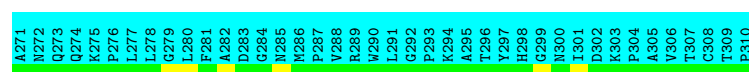
- Molecule 2: Alkaline phosphatase

Chain E:  100%



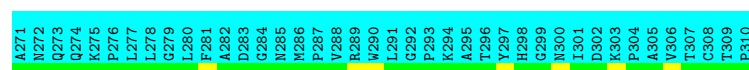
- Molecule 2: Alkaline phosphatase

Chain F:  100%



- Molecule 2: Alkaline phosphatase

Chain G:  100%



- Molecule 2: Alkaline phosphatase

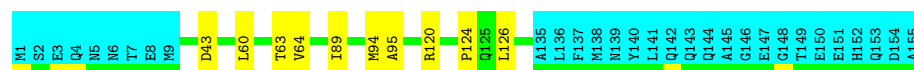
Chain H:  100%



#### 4.2.9 Score per residue for model 9

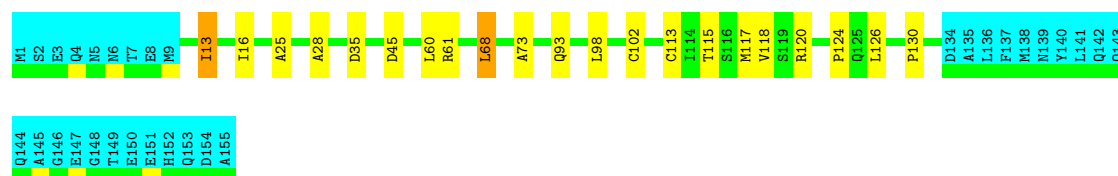
- Molecule 1: Protein-export protein SecB

Chain A:  74% 6% 19%



- Molecule 1: Protein-export protein SecB

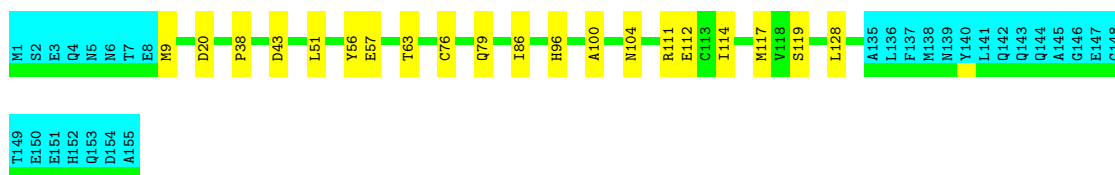
Chain B:  66% 12% 20%



- Molecule 1: Protein-export protein SecB

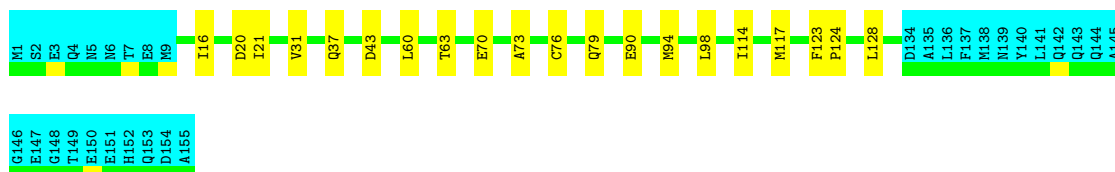
Chain C:  68% 13% 19%





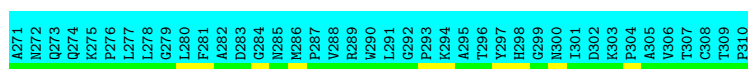
- Molecule 1: Protein-export protein SecB

Chain D: 67% 13% 20%



- Molecule 2: Alkaline phosphatase

Chain E: 100%



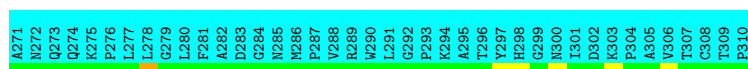
- Molecule 2: Alkaline phosphatase

Chain F: 100%



- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

Chain H: 100%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Protein-export protein SecB

Chain A: 74% 6% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 74% 5% 20%



- Molecule 1: Protein-export protein SecB

Chain C: 74% 7% 19%



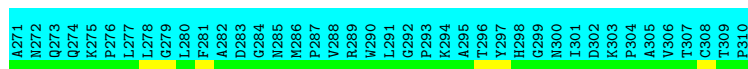
- Molecule 1: Protein-export protein SecB

Chain D: 68% 10% 20%



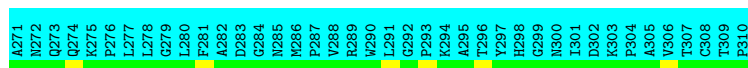
- Molecule 2: Alkaline phosphatase

Chain E: 100%



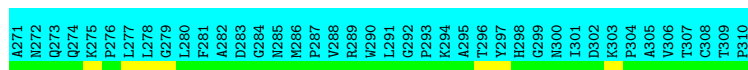
- Molecule 2: Alkaline phosphatase

Chain F: 100%



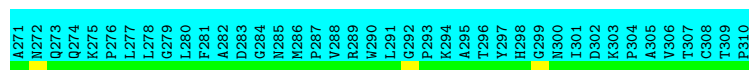
- Molecule 2: Alkaline phosphatase

Chain G: 100%



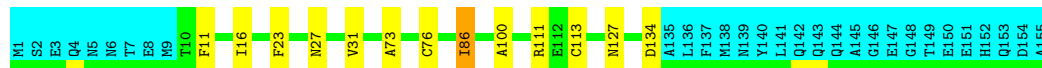
- Molecule 2: Alkaline phosphatase

Chain H: 100%

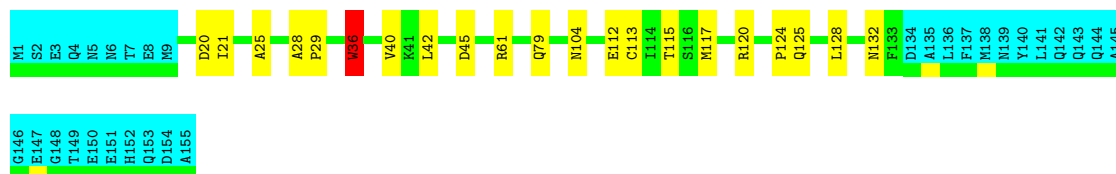


#### 4.2.11 Score per residue for model 11

- Molecule 1: Protein-export protein SecB



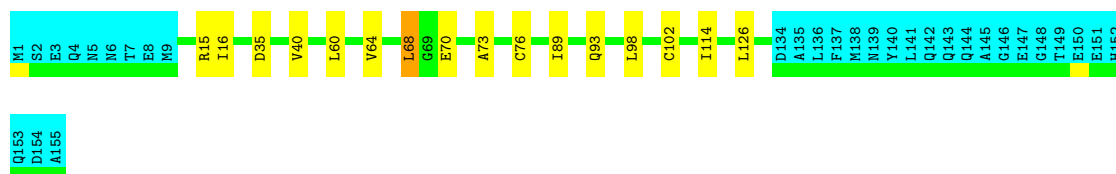
- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB



- Molecule 1: Protein-export protein SecB

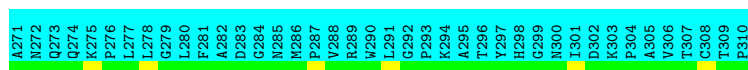


- Molecule 2: Alkaline phosphatase



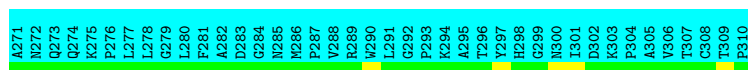
- Molecule 2: Alkaline phosphatase





- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

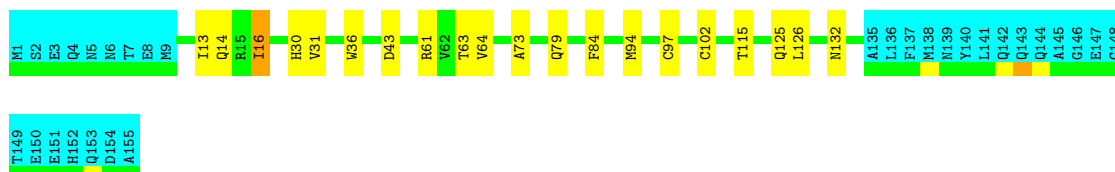
Chain H: 100%



#### 4.2.12 Score per residue for model 12

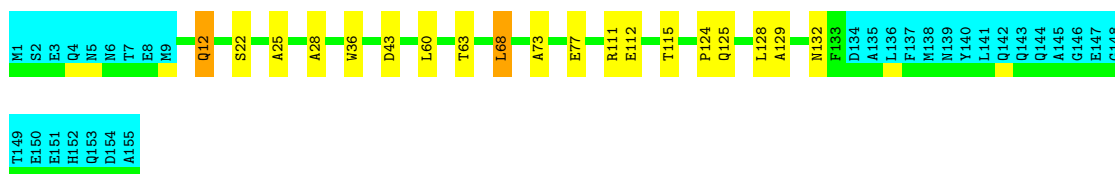
- Molecule 1: Protein-export protein SecB

Chain A: 68% 12% 19%



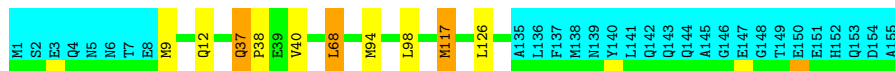
- Molecule 1: Protein-export protein SecB

Chain B: 68% 11% 20%



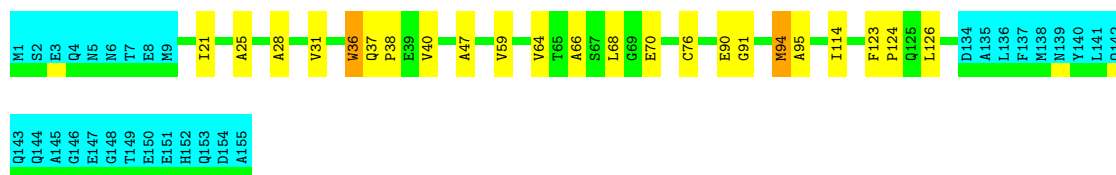
- Molecule 1: Protein-export protein SecB

Chain C: 75% 5% 19%



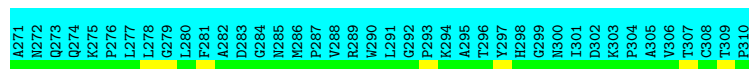
- Molecule 1: Protein-export protein SecB

Chain D: 65% 14% 20%



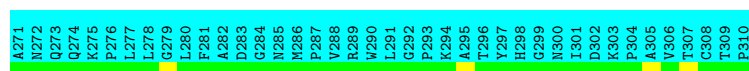
- Molecule 2: Alkaline phosphatase

Chain E: 100%



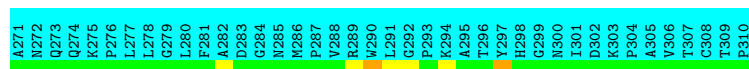
- Molecule 2: Alkaline phosphatase

Chain F: 100%



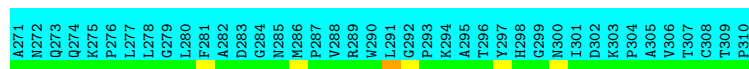
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

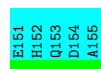
Chain H: 100%



#### 4.2.13 Score per residue for model 13

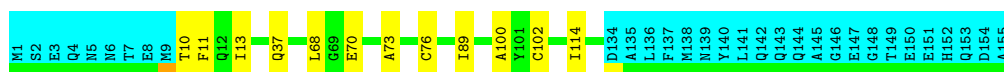
- Molecule 1: Protein-export protein SecB

Chain A: 69% 11% 19%

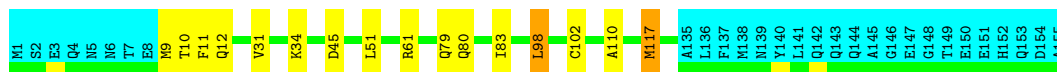


- Molecule 1: Protein-export protein SecB

Chain B: 72% 8% 20%



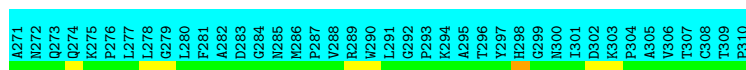
- Molecule 1: Protein-export protein SecB



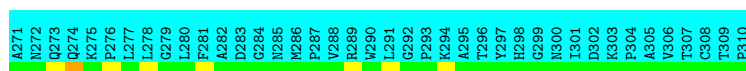
- Molecule 1: Protein-export protein SecB



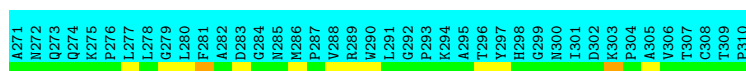
- Molecule 2: Alkaline phosphatase



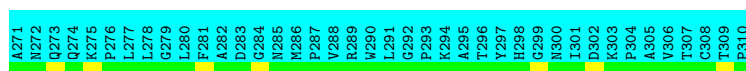
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

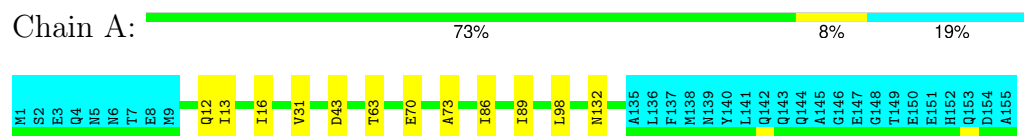


- Molecule 2: Alkaline phosphatase

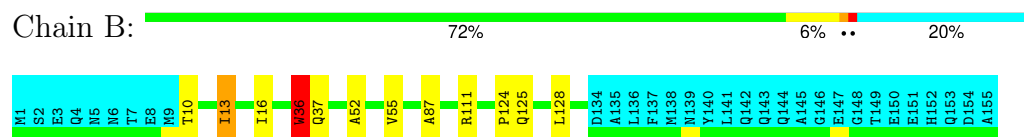


#### 4.2.14 Score per residue for model 14

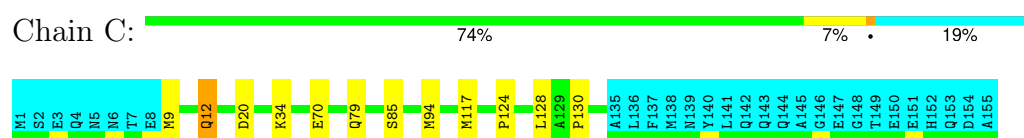
- Molecule 1: Protein-export protein SecB



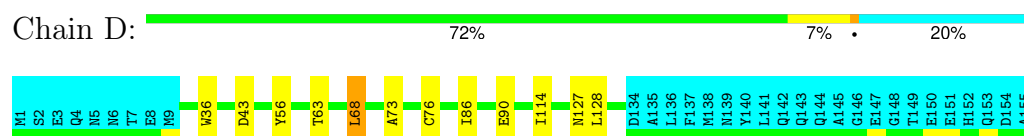
- Molecule 1: Protein-export protein SecB



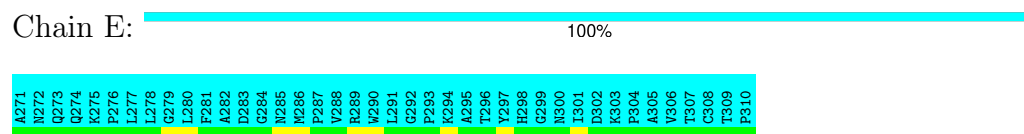
- Molecule 1: Protein-export protein SecB



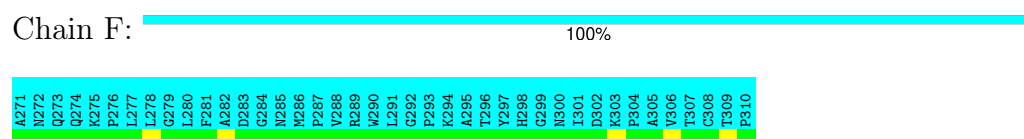
- Molecule 1: Protein-export protein SecB



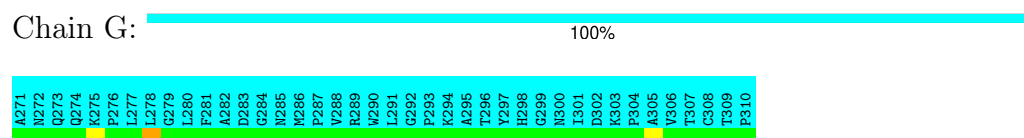
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

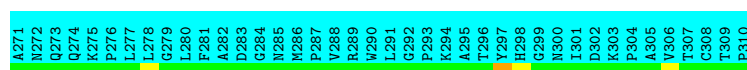


- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase





#### 4.2.15 Score per residue for model 15

- Molecule 1: Protein-export protein SecB

Chain A: 70% 11% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 68% 10% 20%



- Molecule 1: Protein-export protein SecB

Chain C: 76% 19%



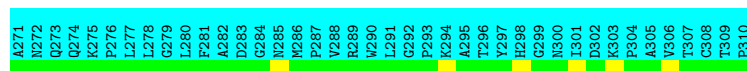
- Molecule 1: Protein-export protein SecB

Chain D: 72% 8% 20%



- Molecule 2: Alkaline phosphatase

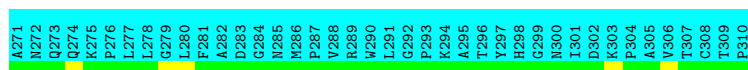
Chain E: 100%



- Molecule 2: Alkaline phosphatase

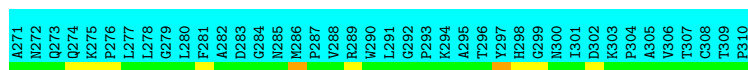
Chain F: 100%





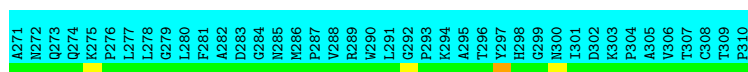
- Molecule 2: Alkaline phosphatase

Chain G: 100%



- Molecule 2: Alkaline phosphatase

Chain H: 100%



#### 4.2.16 Score per residue for model 16

- Molecule 1: Protein-export protein SecB

Chain A: 70% 11% 19%



- Molecule 1: Protein-export protein SecB

Chain B: 71% 9% 20%



- Molecule 1: Protein-export protein SecB

Chain C: 71% 10% 19%



- Molecule 1: Protein-export protein SecB

Chain D: 68% 11% 20%



E150  
E151  
H152  
Q153  
D154  
A155

- Molecule 2: Alkaline phosphatase

Chain E:

100%

A271 N272 N273 Q274 Q275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 N286 P287 V288 V289 R289 L291 G292 P293 K294 A295 T296 Y297 H298 G299 N300 I301 D302 K303 P304 A305 V306 T307 C308 T309 P310

- Molecule 2: Alkaline phosphatase

Chain F:

100%

A271 N272 N273 Q274 Q275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 N286 P287 V288 V289 R289 L291 G292 P293 K294 A295 T296 Y297 H298 G299 N300 I301 D302 K303 P304 A305 V306 T307 C308 T309 P310

- Molecule 2: Alkaline phosphatase

Chain G:

100%

A271 N272 N273 Q274 Q275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 N286 P287 V288 V289 R289 L291 G292 P293 K294 A295 T296 Y297 H298 G299 N300 I301 D302 K303 P304 A305 V306 T307 C308 T309 P310

- Molecule 2: Alkaline phosphatase

Chain H:

100%

A271 N272 N273 Q274 Q275 P276 L277 L278 G279 L280 F281 A282 D283 G284 N285 N286 P287 V288 V289 R289 L291 G292 P293 K294 A295 T296 Y297 H298 G299 N300 I301 D302 K303 P304 A305 V306 T307 C308 T309 P310

#### 4.2.17 Score per residue for model 17

- Molecule 1: Protein-export protein SecB

Chain A:

64%

16%

19%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 I13 I16 F23 E39 D43 L44 D45 A52 R61 V62 T63 V64 F64 A87 E90 Q93 M94 A95 H96 A100 I105 Y109 T115 P124 Q125 L126 N132 F133 D134 A135 L136 F137 M138

H139 Y140 L141 Q142 Q143 Q144 A145 G146 E147 G148 T149 E150 E151 H152 Q153 D154 A155

- Molecule 1: Protein-export protein SecB

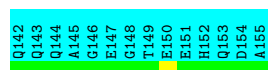
Chain B:

65%

15%

20%

M1 S2 E3 Q4 N5 N6 T7 E8 M9 T10 F11 Q12 R15 D20 I21 A25 A28 P29 H30 Q33 W36 L42 D43 L44 L60 T63 L68 E71 M94 L98 G113 M117 R120 L128 D134 A135 L136 F137 M138 M139 Y140 L141



- Molecule 1: Protein-export protein SecB

Chain C: 70% 9% 19%



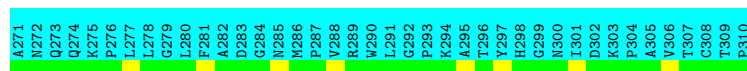
- Molecule 1: Protein-export protein SecB

Chain D: 70% 10% 20%



- Molecule 2: Alkaline phosphatase

Chain E: 100%



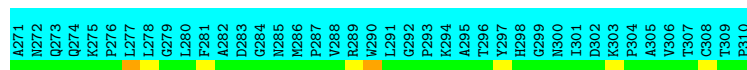
- Molecule 2: Alkaline phosphatase

Chain F: 100%



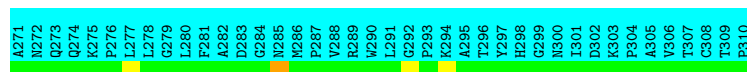
- Molecule 2: Alkaline phosphatase

Chain G: 100%



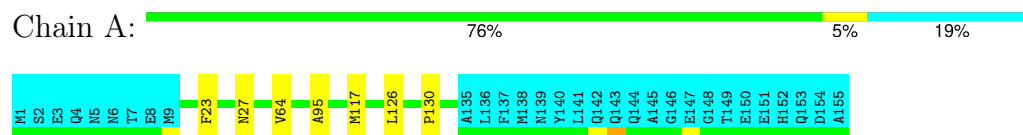
- Molecule 2: Alkaline phosphatase

Chain H: 100%

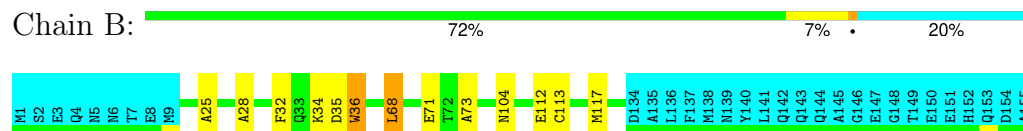


### 4.2.18 Score per residue for model 18

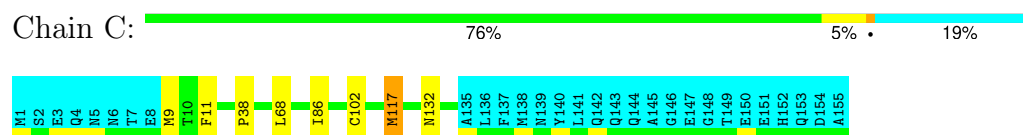
- Molecule 1: Protein-export protein SecB



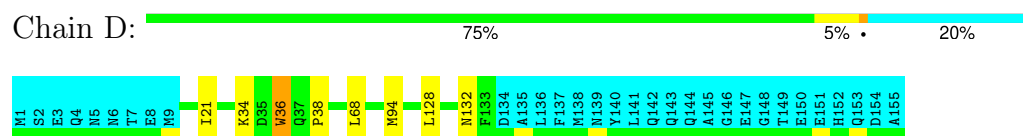
- Molecule 1: Protein-export protein SecB



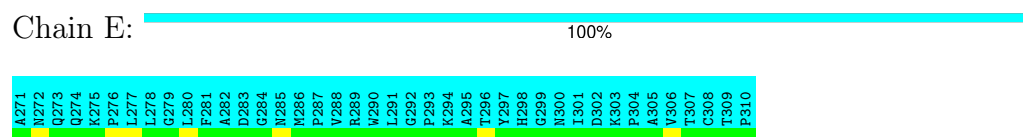
- Molecule 1: Protein-export protein SecB



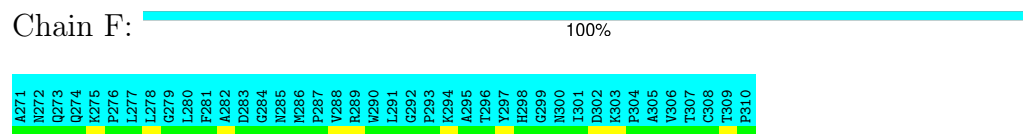
- Molecule 1: Protein-export protein SecB



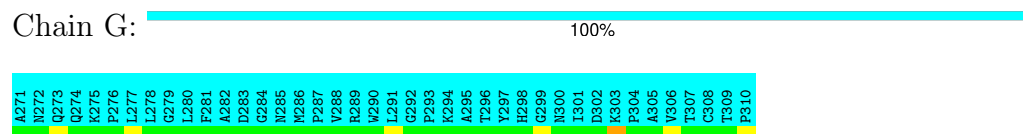
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

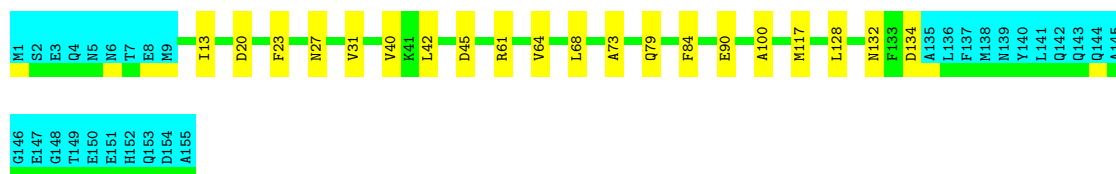
Chain H:  100%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Protein-export protein SecB

Chain A:  68% 13% 19%



- Molecule 1: Protein-export protein SecB

Chain B:  71% 9% 20%



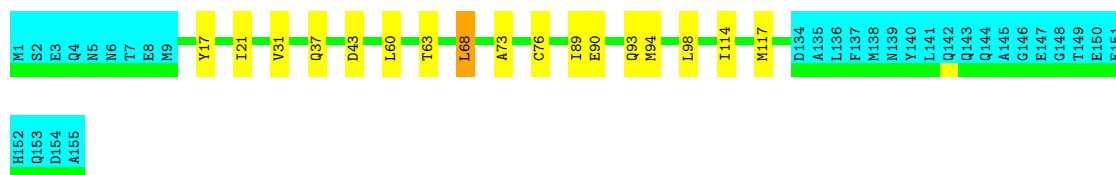
- Molecule 1: Protein-export protein SecB

Chain C:  75% 6% 19%



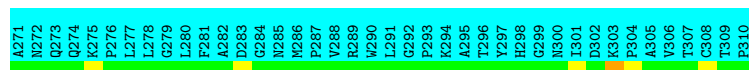
- Molecule 1: Protein-export protein SecB

Chain D:  69% 10% 20%

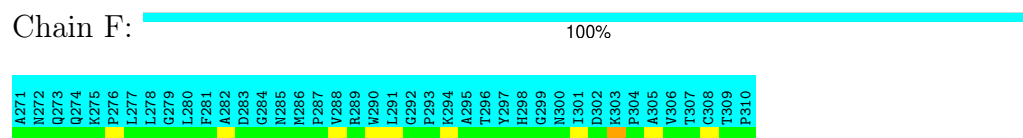


- Molecule 2: Alkaline phosphatase

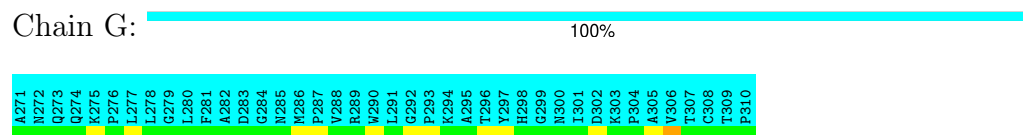
Chain E:  100%



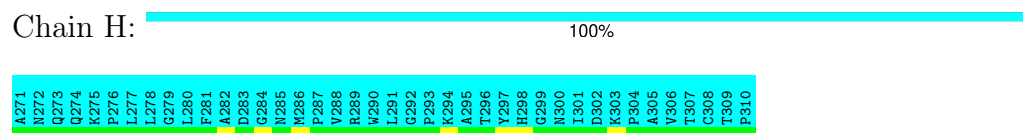
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase

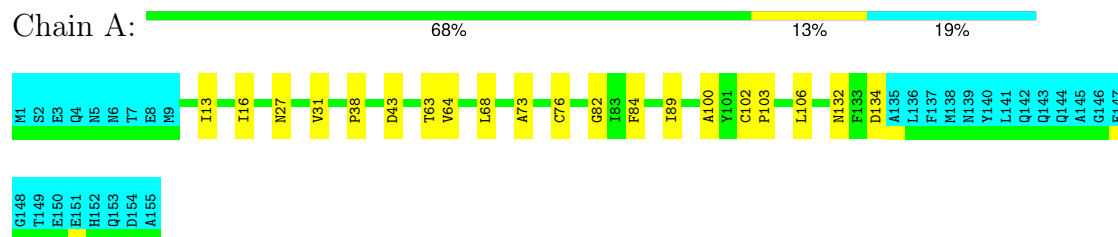


- Molecule 2: Alkaline phosphatase

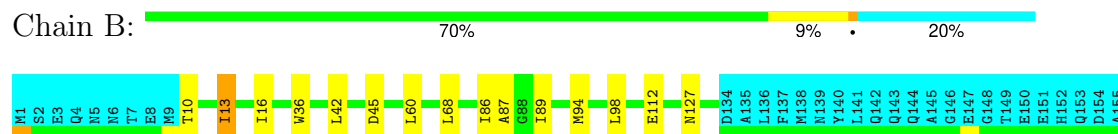


#### 4.2.20 Score per residue for model 20

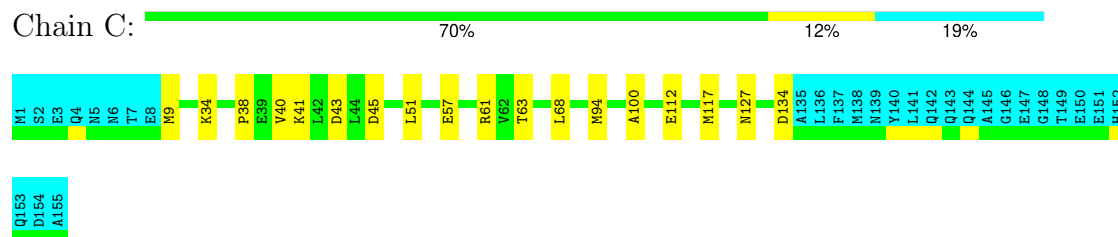
- Molecule 1: Protein-export protein SecB



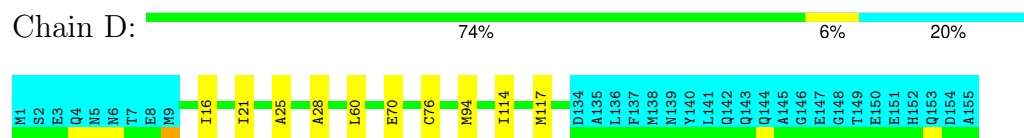
- Molecule 1: Protein-export protein SecB



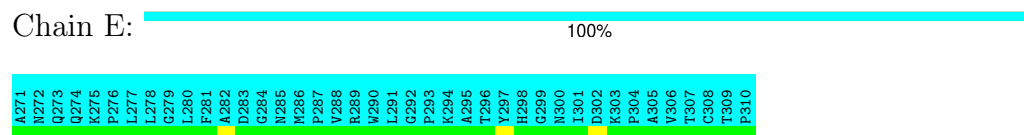
- Molecule 1: Protein-export protein SecB



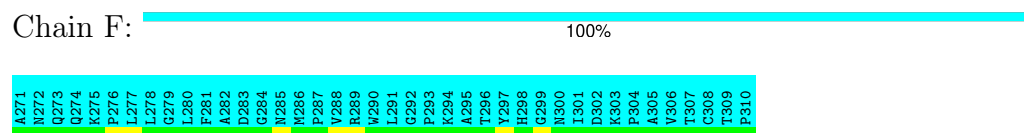
- Molecule 1: Protein-export protein SecB



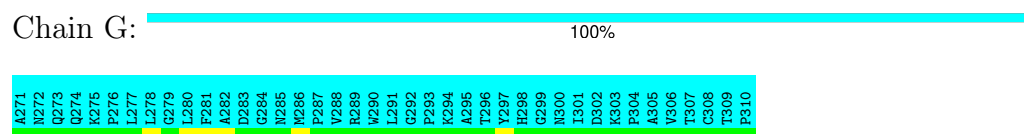
- Molecule 2: Alkaline phosphatase



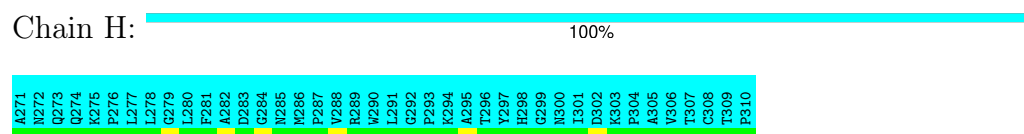
- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase



- Molecule 2: Alkaline phosphatase



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	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	8
Total number of shifts	5072
Number of shifts mapped to atoms	5072
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	53%



## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	973	946	944	7±2
1	B	965	942	940	7±2
1	C	981	955	953	6±3
1	D	965	942	940	6±2
2	E	0	0	0	0±0
2	F	0	0	0	0±0
2	G	0	0	0	0±0
2	H	0	0	0	0±0
All	All	77680	75700	75540	460

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:ALA:HB1	1:B:28:ALA:HB2	0.84	1.47	15	8
1:A:31:VAL:HG21	1:A:73:ALA:HA	0.67	1.65	13	11
1:A:64:VAL:HG11	1:A:126:LEU:HD21	0.65	1.68	12	8
1:D:25:ALA:HB1	1:D:28:ALA:HB2	0.64	1.68	13	3
1:B:25:ALA:CB	1:B:28:ALA:HB2	0.62	2.24	19	11
1:D:40:VAL:HG12	1:D:66:ALA:HB2	0.62	1.72	12	1
1:C:43:ASP:HB2	1:C:63:THR:HB	0.61	1.72	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:PHE:HD1	1:A:76:CYS:HG	0.61	1.37	15	3
1:A:100:ALA:HB1	1:A:134:ASP:HA	0.61	1.73	13	8
1:C:9:MET:SD	1:C:11:PHE:HB2	0.60	2.36	8	2
1:B:98:LEU:HA	1:B:102:CYS:SG	0.60	2.36	4	6
1:A:122:THR:HG21	1:B:15:ARG:HD2	0.60	1.73	5	1
1:B:60:LEU:HD11	1:B:103:PRO:HA	0.59	1.74	15	1
1:B:125:GLN:HB2	1:C:124:PRO:HA	0.58	1.75	14	2
1:D:43:ASP:HB2	1:D:63:THR:HB	0.57	1.75	8	7
1:D:68:LEU:HD13	1:D:73:ALA:HB2	0.56	1.76	3	2
1:D:94:MET:SD	1:D:98:LEU:HD23	0.56	2.41	4	1
1:D:76:CYS:SG	1:D:114:ILE:HG23	0.56	2.40	14	13
1:C:45:ASP:HB3	1:C:61:ARG:HB2	0.56	1.77	13	2
1:D:38:PRO:HB3	1:D:68:LEU:HD11	0.55	1.77	13	1
1:C:61:ARG:HG2	1:C:79:GLN:HG2	0.55	1.77	2	3
1:A:60:LEU:HD23	1:A:106:LEU:HD12	0.55	1.79	3	2
1:A:122:THR:HG21	1:D:125:GLN:HE21	0.55	1.60	13	1
1:B:61:ARG:HB2	1:B:79:GLN:HG2	0.55	1.79	3	1
1:C:98:LEU:HA	1:C:102:CYS:SG	0.55	2.42	3	4
1:D:42:LEU:HD12	1:D:128:LEU:HD12	0.55	1.78	7	1
1:A:43:ASP:HB2	1:A:63:THR:HB	0.54	1.79	17	13
1:A:61:ARG:HB2	1:A:79:GLN:HG2	0.53	1.79	19	3
1:B:11:PHE:HE1	1:B:102:CYS:HG	0.53	1.42	6	4
1:C:20:ASP:HB3	1:C:79:GLN:HB2	0.53	1.80	17	5
1:C:117:MET:HE3	1:D:21:ILE:HD13	0.53	1.78	6	4
1:C:34:LYS:HD2	1:C:68:LEU:HD21	0.52	1.81	4	2
1:B:86:ILE:HB	1:B:89:ILE:HD11	0.52	1.82	5	2
1:C:45:ASP:HB3	1:C:61:ARG:HD2	0.52	1.81	17	1
1:B:18:THR:HG21	1:B:21:ILE:HD11	0.52	1.82	3	1
1:B:43:ASP:HB2	1:B:63:THR:HB	0.52	1.81	12	2
1:D:68:LEU:HG	1:D:73:ALA:HB2	0.52	1.80	2	6
1:A:44:LEU:HD21	1:A:60:LEU:HD12	0.52	1.81	6	1
1:A:82:GLY:HA3	1:A:106:LEU:HD21	0.52	1.80	6	3
1:B:115:THR:HG23	1:B:125:GLN:HB2	0.52	1.80	11	4
1:D:31:VAL:HG21	1:D:73:ALA:HA	0.52	1.80	9	2
1:D:20:ASP:HB3	1:D:79:GLN:HB2	0.51	1.81	16	3
1:B:21:ILE:HD11	1:B:113:CYS:SG	0.51	2.46	3	7
1:C:94:MET:HG2	1:C:98:LEU:HD23	0.51	1.81	1	1
1:A:120:ARG:HD3	1:B:113:CYS:SG	0.51	2.46	6	3
1:B:68:LEU:HG	1:B:73:ALA:HB2	0.51	1.82	9	5
1:B:36:TRP:HA	1:B:36:TRP:CE3	0.51	2.41	11	4
1:D:76:CYS:SG	1:D:114:ILE:HG12	0.50	2.46	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:61:ARG:HB2	1:D:79:GLN:HG2	0.50	1.83	8	1
1:A:13:ILE:HG21	1:C:130:PRO:HG2	0.50	1.83	14	3
1:C:34:LYS:HE3	1:C:71:GLU:HG3	0.50	1.83	5	2
1:C:76:CYS:SG	1:C:114:ILE:HA	0.50	2.46	5	2
1:B:52:ALA:HB3	1:B:55:VAL:HB	0.50	1.82	14	1
1:C:51:LEU:HD11	1:C:83:ILE:HD12	0.50	1.83	5	6
1:C:27:ASN:HB2	1:C:30:HIS:HB3	0.50	1.81	3	1
1:C:111:ARG:HG3	1:C:128:LEU:HB2	0.50	1.83	9	1
1:B:13:ILE:HD11	1:B:16:ILE:HG13	0.49	1.84	8	4
1:C:10:THR:HG22	1:C:12:GLN:HE22	0.49	1.67	13	1
1:C:9:MET:SD	1:C:97:CYS:SG	0.49	3.07	11	2
1:B:45:ASP:HB3	1:B:61:ARG:HD3	0.49	1.84	11	1
1:A:25:ALA:HB1	1:A:28:ALA:HB2	0.49	1.85	2	2
1:A:11:PHE:HE2	1:A:84:PHE:HB3	0.48	1.68	5	4
1:A:20:ASP:HB2	1:A:79:GLN:HB2	0.48	1.84	19	1
1:B:10:THR:HG22	1:B:12:GLN:HE22	0.48	1.67	10	1
1:C:11:PHE:HE1	1:C:102:CYS:HG	0.48	1.50	18	2
1:A:109:TYR:CE1	1:C:108:PRO:HA	0.48	2.43	17	1
1:B:64:VAL:HG21	1:B:114:ILE:HG21	0.48	1.83	4	2
1:D:38:PRO:HA	1:D:68:LEU:HB3	0.48	1.86	1	2
1:A:51:LEU:HD11	1:A:57:GLU:HB2	0.48	1.86	2	3
1:C:11:PHE:CE1	1:C:102:CYS:SG	0.48	3.06	3	1
1:D:36:TRP:CD2	1:D:68:LEU:HD22	0.48	2.43	16	1
1:B:12:GLN:NE2	1:B:85:SER:HB2	0.48	2.24	16	1
1:A:68:LEU:HD13	1:A:73:ALA:HB2	0.47	1.86	20	2
1:C:11:PHE:HE1	1:C:102:CYS:SG	0.47	2.32	13	1
1:C:117:MET:HE2	1:D:21:ILE:HG21	0.47	1.86	18	5
1:B:111:ARG:HG3	1:B:128:LEU:HB3	0.47	1.85	14	1
1:C:100:ALA:HB1	1:C:134:ASP:HA	0.47	1.85	16	3
1:C:40:VAL:HG21	1:C:126:LEU:HD11	0.47	1.85	12	1
1:C:45:ASP:HB2	1:C:61:ARG:HB3	0.47	1.86	10	2
1:A:64:VAL:HB	1:A:76:CYS:HB2	0.47	1.86	20	2
1:C:96:HIS:O	1:C:100:ALA:HB3	0.47	2.10	9	3
1:C:51:LEU:HD11	1:C:57:GLU:HB2	0.47	1.86	15	4
1:D:21:ILE:HG23	1:D:78:VAL:HG22	0.47	1.86	15	1
1:C:86:ILE:HD12	1:C:94:MET:SD	0.47	2.50	16	1
1:A:113:CYS:SG	1:B:120:ARG:HD3	0.47	2.50	11	2
1:B:68:LEU:HD23	1:B:73:ALA:HB2	0.46	1.86	16	1
1:B:13:ILE:HD12	1:D:127:ASN:HB3	0.46	1.87	14	1
1:B:11:PHE:HE1	1:B:102:CYS:SG	0.46	2.33	6	2
1:A:86:ILE:HD13	1:A:98:LEU:HD21	0.46	1.87	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:THR:HB	1:B:87:ALA:HB3	0.46	1.88	14	3
1:D:96:HIS:O	1:D:100:ALA:HB3	0.46	2.11	15	1
1:D:98:LEU:HA	1:D:102:CYS:SG	0.46	2.51	2	2
1:D:47:ALA:HB3	1:D:59:VAL:HB	0.46	1.87	8	4
1:C:34:LYS:HE2	1:C:73:ALA:HA	0.46	1.86	5	5
1:B:34:LYS:HB3	1:B:68:LEU:HB2	0.46	1.87	1	1
1:A:17:TYR:HB3	1:B:122:THR:HG23	0.46	1.88	7	1
1:B:42:LEU:HD12	1:B:128:LEU:HD11	0.46	1.88	10	1
1:B:33:GLN:HG3	1:B:34:LYS:HG3	0.45	1.88	5	1
1:A:20:ASP:HB3	1:A:79:GLN:HB2	0.45	1.87	7	1
1:D:11:PHE:HE2	1:D:102:CYS:HG	0.45	1.53	10	1
1:B:22:SER:HB2	1:B:77:GLU:HB3	0.45	1.88	12	1
1:C:12:GLN:HG2	1:C:85:SER:HB3	0.45	1.89	5	1
1:D:23:PHE:HB2	1:D:117:MET:SD	0.45	2.52	1	1
1:D:21:ILE:CG2	1:D:117:MET:SD	0.45	3.04	17	8
1:A:104:ASN:ND2	1:A:134:ASP:HB2	0.45	2.27	5	1
1:A:13:ILE:HG12	1:A:84:PHE:HD2	0.45	1.71	8	6
1:C:62:VAL:HB	1:C:114:ILE:HD11	0.45	1.88	4	2
1:A:96:HIS:O	1:A:100:ALA:HB3	0.45	2.12	17	1
1:D:56:TYR:HB2	1:D:86:ILE:HD13	0.45	1.87	16	3
1:C:68:LEU:HD23	1:C:68:LEU:H	0.45	1.71	17	1
1:A:40:VAL:HA	1:A:65:THR:O	0.44	2.12	8	1
1:D:36:TRP:CH2	1:D:68:LEU:HD13	0.44	2.46	10	1
1:D:38:PRO:HA	1:D:68:LEU:HD11	0.44	1.89	12	2
1:B:64:VAL:HG11	1:B:126:LEU:HD21	0.44	1.88	3	1
1:D:64:VAL:HG11	1:D:126:LEU:HD13	0.44	1.87	17	1
1:A:94:MET:SD	1:A:95:ALA:N	0.44	2.90	9	1
1:B:38:PRO:HB3	1:B:68:LEU:HD21	0.44	1.88	16	1
1:C:113:CYS:O	1:C:117:MET:SD	0.44	2.76	6	3
1:A:28:ALA:HB3	1:A:29:PRO:HD3	0.44	1.90	3	1
1:A:76:CYS:HB3	1:A:114:ILE:HG23	0.44	1.89	4	1
1:C:13:ILE:HD13	1:C:13:ILE:H	0.44	1.73	6	1
1:D:64:VAL:HB	1:D:76:CYS:HB2	0.44	1.88	15	1
1:A:23:PHE:HB2	1:A:117:MET:SD	0.44	2.53	8	4
1:A:94:MET:SD	1:A:98:LEU:HD21	0.44	2.53	2	1
1:B:34:LYS:HB2	1:B:68:LEU:HD13	0.44	1.90	6	2
1:B:111:ARG:HG3	1:B:128:LEU:HB2	0.44	1.90	12	1
1:D:111:ARG:HD3	1:D:128:LEU:O	0.44	2.13	8	3
1:D:123:PHE:HB3	1:D:124:PRO:HD2	0.44	1.89	12	2
1:C:80:GLN:HB2	1:C:110:ALA:HB2	0.44	1.89	13	1
1:A:122:THR:HB	1:B:15:ARG:HH21	0.43	1.73	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ILE:HD12	1:C:130:PRO:HG3	0.43	1.90	1	1
1:B:31:VAL:HG21	1:B:73:ALA:HA	0.43	1.90	1	1
1:B:34:LYS:O	1:B:68:LEU:HD22	0.43	2.13	4	1
1:B:42:LEU:HD21	1:B:128:LEU:HD11	0.43	1.89	3	2
1:B:60:LEU:HD22	1:B:103:PRO:HA	0.43	1.90	4	1
1:A:115:THR:HG23	1:A:125:GLN:HG3	0.43	1.90	4	4
1:B:57:GLU:HG2	1:B:83:ILE:HG12	0.43	1.90	15	1
1:C:45:ASP:HB3	1:C:61:ARG:HB3	0.43	1.89	20	2
1:A:94:MET:C	1:A:94:MET:SD	0.43	2.97	10	1
1:A:13:ILE:HG12	1:A:84:PHE:CD2	0.43	2.48	19	2
1:B:76:CYS:SG	1:B:114:ILE:HA	0.43	2.53	13	2
1:D:111:ARG:HH12	1:D:130:PRO:HB3	0.43	1.74	8	1
1:C:12:GLN:NE2	1:C:85:SER:HB2	0.43	2.28	14	1
1:D:56:TYR:HB2	1:D:86:ILE:HD12	0.43	1.90	14	1
1:B:125:GLN:HE21	1:B:125:GLN:HA	0.43	1.73	6	1
1:A:34:LYS:HG3	1:A:71:GLU:HG2	0.43	1.89	2	1
1:B:30:HIS:O	1:B:33:GLN:HG2	0.43	2.13	7	2
1:B:113:CYS:O	1:B:117:MET:HG2	0.43	2.14	15	4
1:B:42:LEU:HD22	1:B:128:LEU:HD21	0.43	1.90	11	1
1:B:64:VAL:HG23	1:B:114:ILE:HD13	0.43	1.91	19	1
1:A:45:ASP:HB2	1:A:61:ARG:HB3	0.43	1.90	1	2
1:C:120:ARG:HD3	1:D:113:CYS:SG	0.43	2.54	3	1
1:B:130:PRO:HG3	1:D:16:ILE:HD12	0.42	1.89	1	1
1:D:94:MET:SD	1:D:98:LEU:HD12	0.42	2.53	1	1
1:B:94:MET:O	1:B:98:LEU:HG	0.42	2.13	2	1
1:B:64:VAL:CG2	1:B:114:ILE:HD13	0.42	2.43	19	1
1:D:27:ASN:ND2	1:D:72:THR:HB	0.42	2.29	8	1
1:A:45:ASP:HB3	1:A:61:ARG:HB3	0.42	1.91	19	1
1:B:27:ASN:ND2	1:B:71:GLU:HB2	0.42	2.29	4	1
1:C:9:MET:HA	1:C:89:ILE:HD12	0.42	1.90	5	1
1:C:34:LYS:HE3	1:C:73:ALA:HA	0.42	1.90	11	1
1:A:16:ILE:HD12	1:A:16:ILE:N	0.42	2.29	12	1
1:A:105:ILE:HD11	1:C:132:ASN:HD21	0.42	1.73	17	1
1:B:117:MET:SD	1:B:120:ARG:HD2	0.42	2.55	9	2
1:C:37:GLN:N	1:C:38:PRO:HD3	0.42	2.30	12	1
1:C:38:PRO:HA	1:C:68:LEU:HB3	0.42	1.92	12	1
1:A:102:CYS:N	1:A:103:PRO:HD2	0.42	2.29	6	3
1:B:45:ASP:HB3	1:B:61:ARG:HB3	0.42	1.92	6	2
1:C:42:LEU:HG	1:C:128:LEU:HD21	0.42	1.91	8	1
1:C:89:ILE:HD13	1:C:94:MET:HA	0.42	1.91	8	1
1:B:42:LEU:HD11	1:B:128:LEU:HD21	0.42	1.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD21	1:A:103:PRO:HB3	0.42	1.92	3	1
1:D:34:LYS:HE2	1:D:36:TRP:HE1	0.42	1.74	18	1
1:C:38:PRO:HG2	1:C:40:VAL:HG13	0.42	1.92	20	1
1:D:16:ILE:H	1:D:16:ILE:HD13	0.42	1.75	3	1
1:A:31:VAL:HG11	1:A:73:ALA:HA	0.42	1.92	6	1
1:B:105:ILE:HG23	1:D:111:ARG:NH2	0.42	2.29	15	1
1:C:12:GLN:HG2	1:C:85:SER:HB2	0.42	1.92	17	1
1:A:13:ILE:CD1	1:A:105:ILE:HG21	0.42	2.45	3	1
1:D:38:PRO:HB3	1:D:68:LEU:HD23	0.42	1.91	4	1
1:A:14:GLN:HA	1:A:14:GLN:HE21	0.42	1.75	8	1
1:A:10:THR:HB	1:A:87:ALA:HB3	0.42	1.90	17	1
1:A:23:PHE:O	1:B:20:ASP:HA	0.42	2.14	17	1
1:B:34:LYS:NZ	1:B:71:GLU:HG2	0.42	2.30	18	1
1:A:13:ILE:HD11	1:A:105:ILE:HG21	0.42	1.91	16	1
1:B:110:ALA:O	1:B:114:ILE:HG13	0.42	2.15	19	1
1:B:28:ALA:HB3	1:B:29:PRO:HD3	0.42	1.92	2	1
1:A:111:ARG:NH1	1:C:105:ILE:HD12	0.42	2.30	11	1
1:B:30:HIS:HB3	1:B:33:GLN:NE2	0.42	2.30	17	1
1:A:16:ILE:HD13	1:C:130:PRO:HG3	0.41	1.91	6	1
1:A:56:TYR:HB2	1:A:86:ILE:HD13	0.41	1.91	15	1
1:A:40:VAL:HG23	1:A:64:VAL:HG13	0.41	1.91	19	1
1:B:68:LEU:HD12	1:B:73:ALA:HB2	0.41	1.91	13	1
1:A:97:CYS:SG	1:A:102:CYS:SG	0.41	3.18	12	1
1:D:60:LEU:HD23	1:D:106:LEU:HD12	0.41	1.91	4	1
1:B:118:VAL:HG21	1:B:126:LEU:HD23	0.41	1.92	9	1
1:D:64:VAL:HG11	1:D:126:LEU:HD11	0.41	1.92	11	1
1:D:38:PRO:HA	1:D:68:LEU:HD21	0.41	1.92	16	1
1:B:32:PHE:HA	1:B:35:ASP:HB2	0.41	1.92	18	1
1:A:130:PRO:HD3	1:C:13:ILE:HG22	0.41	1.92	5	1
1:B:89:ILE:HD12	1:B:94:MET:HA	0.41	1.93	20	1
1:D:25:ALA:CB	1:D:28:ALA:HB2	0.41	2.44	20	1
1:A:17:TYR:HE2	1:B:28:ALA:HB1	0.41	1.75	7	1
1:C:56:TYR:HB2	1:C:86:ILE:HD13	0.41	1.92	9	1
1:A:127:ASN:HB2	1:C:13:ILE:HD13	0.41	1.92	11	1
1:B:118:VAL:HG21	1:B:126:LEU:HD13	0.41	1.93	7	1
1:D:43:ASP:HB3	1:D:63:THR:HB	0.41	1.92	9	1
1:C:104:ASN:ND2	1:C:134:ASP:HB2	0.41	2.30	16	1
1:C:21:ILE:HG12	1:C:113:CYS:SG	0.41	2.56	17	1
1:C:28:ALA:HB1	1:D:17:TYR:HE2	0.41	1.76	19	1
1:D:94:MET:SD	1:D:95:ALA:N	0.41	2.94	12	1
1:D:31:VAL:HG13	1:D:68:LEU:HD11	0.41	1.92	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:CYS:HA	1:A:101:TYR:HB3	0.40	1.92	13	1
1:B:34:LYS:HB3	1:B:68:LEU:HB3	0.40	1.91	8	1
1:B:20:ASP:HB3	1:B:79:GLN:HB2	0.40	1.93	11	1
1:A:34:LYS:HD3	1:A:35:ASP:N	0.40	2.32	15	1
1:A:52:ALA:HB3	1:A:55:VAL:HB	0.40	1.92	15	1
1:C:9:MET:SD	1:C:89:ILE:HD13	0.40	2.57	2	1
1:B:125:GLN:NE2	1:B:127:ASN:HD21	0.40	2.13	8	1
1:D:31:VAL:HG22	1:D:36:TRP:CZ2	0.40	2.51	12	1
1:A:92:THR:HA	1:A:95:ALA:HB3	0.40	1.91	1	1
1:C:68:LEU:N	1:C:68:LEU:HD12	0.40	2.31	2	1
1:B:19:LYS:HD2	1:B:81:GLY:HA3	0.40	1.93	5	1
1:A:11:PHE:HA	1:A:86:ILE:HG22	0.40	1.93	11	1
1:D:51:LEU:HD11	1:D:57:GLU:HB2	0.40	1.92	3	1
1:D:15:ARG:HA	1:D:15:ARG:NE	0.40	2.31	4	1
1:A:86:ILE:HG21	1:A:97:CYS:SG	0.40	2.56	6	1
1:C:41:LYS:HE3	1:C:43:ASP:HB2	0.40	1.93	6	1
1:B:115:THR:HG21	1:C:119:SER:OG	0.40	2.16	9	1
1:D:40:VAL:HB	1:D:64:VAL:HG13	0.40	1.91	12	1
1:C:31:VAL:HG21	1:C:73:ALA:HA	0.40	1.93	16	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/155 (81%)	118±2 (94±2%)	7±2 (6±2%)	0±0 (0±0%)	100	100
1	B	124/155 (80%)	116±2 (93±1%)	8±2 (6±1%)	1±1 (1±1%)	21	71
1	C	126/155 (81%)	116±1 (92±1%)	9±1 (7±1%)	1±0 (1±0%)	16	65
1	D	124/155 (80%)	117±1 (95±1%)	7±1 (5±1%)	0±0 (0±0%)	45	81
2	E	0	-	-	-	-	-
2	F	0	-	-	-	-	-
2	G	0	-	-	-	-	-
2	H	0	-	-	-	-	-
All	All	9980/15600 (64%)	9340 (94%)	595 (6%)	45 (0%)	27	74

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	9	MET	20
1	B	36	TRP	10
1	B	124	PRO	5
1	C	130	PRO	3
1	B	130	PRO	2
1	D	91	GLY	2
1	D	124	PRO	1
1	C	124	PRO	1
1	D	28	ALA	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	107/132 (81%)	104±2 (97±2%)	3±2 (3±2%)	41	89
1	B	106/132 (80%)	101±2 (96±2%)	5±2 (4±2%)	26	79
1	C	108/132 (82%)	103±1 (95±1%)	5±1 (5±1%)	26	78
1	D	106/132 (80%)	101±2 (95±2%)	5±2 (5±2%)	24	77
2	E	0	-	-	-	-
2	F	0	-	-	-	-
2	G	0	-	-	-	-
2	H	0	-	-	-	-
All	All	8540/13120 (65%)	8190 (96%)	350 (4%)	28	81

All 92 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	C	117	MET	20
1	B	36	TRP	17
1	D	94	MET	12
1	D	70	GLU	12
1	A	16	ILE	10
1	C	68	LEU	10
1	C	34	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	D	36	TRP	10
1	D	68	LEU	10
1	B	112	GLU	10
1	D	90	GLU	9
1	B	68	LEU	9
1	D	16	ILE	8
1	B	60	LEU	8
1	D	60	LEU	8
1	B	13	ILE	8
1	A	89	ILE	7
1	C	89	ILE	7
1	D	128	LEU	6
1	C	112	GLU	6
1	B	98	LEU	5
1	B	104	ASN	5
1	D	37	GLN	5
1	C	13	ILE	5
1	C	127	ASN	4
1	C	128	LEU	4
1	D	34	LYS	4
1	B	12	GLN	4
1	B	37	GLN	4
1	C	94	MET	4
1	A	132	ASN	4
1	A	90	GLU	4
1	C	98	LEU	4
1	C	12	GLN	4
1	A	27	ASN	4
1	A	94	MET	3
1	C	104	ASN	3
1	B	89	ILE	3
1	B	127	ASN	3
1	B	128	LEU	3
1	D	126	LEU	3
1	B	125	GLN	3
1	A	60	LEU	3
1	A	70	GLU	3
1	D	93	GLN	3
1	C	93	GLN	2
1	A	31	VAL	2
1	D	27	ASN	2
1	D	42	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	B	94	MET	2
1	A	128	LEU	2
1	A	14	GLN	2
1	C	42	LEU	2
1	A	86	ILE	2
1	A	68	LEU	2
1	C	31	VAL	2
1	D	98	LEU	2
1	D	76	CYS	1
1	B	126	LEU	1
1	C	125	GLN	1
1	A	37	GLN	1
1	B	113	CYS	1
1	D	125	GLN	1
1	B	42	LEU	1
1	D	15	ARG	1
1	B	41	LYS	1
1	C	33	GLN	1
1	C	133	PHE	1
1	C	38	PRO	1
1	A	44	LEU	1
1	B	29	PRO	1
1	D	89	ILE	1
1	A	30	HIS	1
1	B	132	ASN	1
1	C	37	GLN	1
1	A	43	ASP	1
1	A	56	TYR	1
1	A	79	GLN	1
1	B	70	GLU	1
1	D	39	GLU	1
1	C	70	GLU	1
1	C	111	ARG	1
1	A	39	GLU	1
1	B	11	PHE	1
1	B	44	LEU	1
1	B	71	GLU	1
1	C	60	LEU	1
1	A	130	PRO	1
1	C	86	ILE	1
1	A	42	LEU	1
1	C	77	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	C	41	LYS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 53% for the well-defined parts and 49% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_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	1046
Number of shifts mapped to atoms	1046
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	$0.25 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	128	$0.85 \pm 0.15$	Should be checked
$^{13}\text{C}'$	137	$0.29 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	133	$-1.14 \pm 0.23$	Should be applied

#### 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 13%, i.e. 893 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	459/2467 (19%)	112/998 (11%)	235/998 (24%)	112/471 (24%)
Sidechain	369/3626 (10%)	204/2375 (9%)	165/1139 (14%)	0/112 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	65/576 (11%)	33/280 (12%)	31/276 (11%)	1/20 (5%)
Overall	893/6669 (13%)	349/3653 (10%)	431/2413 (18%)	113/603 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 1046 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	542/3856 (14%)	133/1564 (9%)	276/1560 (18%)	133/732 (18%)
Sidechain	427/5612 (8%)	234/3656 (6%)	193/1768 (11%)	0/188 (0%)
Aromatic	77/840 (9%)	39/408 (10%)	37/392 (9%)	1/40 (2%)
Overall	1046/10308 (10%)	406/5628 (7%)	506/3720 (14%)	134/960 (14%)

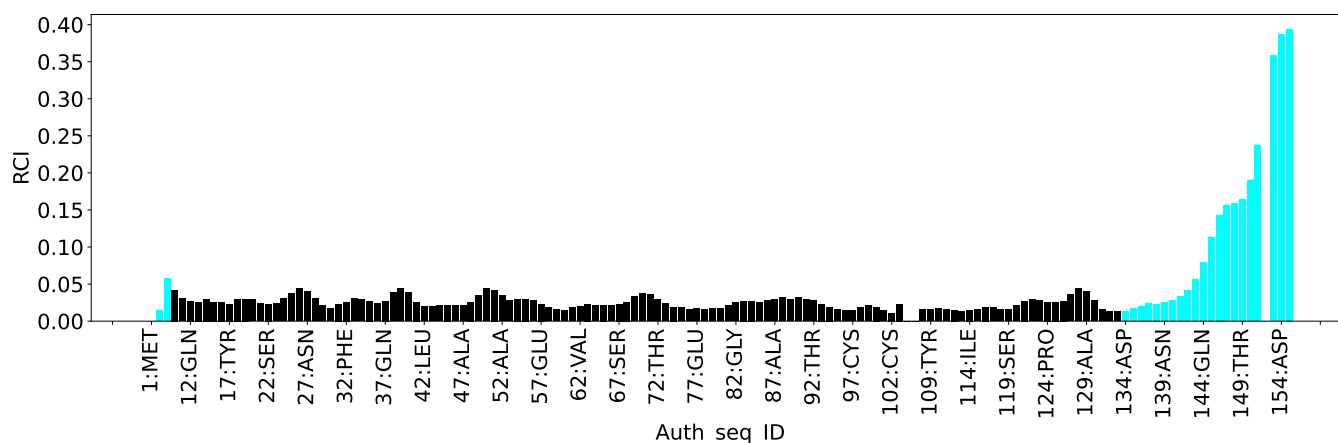
#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

#### 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:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_list\_2*

### 7.2.1 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	1044
Number of shifts mapped to atoms	1044
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

### 7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	$0.28 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	126	$0.79 \pm 0.23$	Should be checked
$^{13}\text{C}'$	135	$0.26 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	132	$-1.09 \pm 0.30$	Should be applied

### 7.2.3 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 13%, i.e. 883 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	452/2467 (18%)	110/998 (11%)	232/998 (23%)	110/471 (23%)
Sidechain	366/3626 (10%)	204/2375 (9%)	162/1139 (14%)	0/112 (0%)
Aromatic	65/576 (11%)	33/280 (12%)	31/276 (11%)	1/20 (5%)
Overall	883/6669 (13%)	347/3653 (9%)	425/2413 (18%)	111/603 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 1044 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	539/3856 (14%)	132/1564 (8%)	275/1560 (18%)	132/732 (18%)
Sidechain	428/5612 (8%)	237/3656 (6%)	191/1768 (11%)	0/188 (0%)
Aromatic	77/840 (9%)	39/408 (10%)	37/392 (9%)	1/40 (2%)
Overall	1044/10308 (10%)	408/5628 (7%)	503/3720 (14%)	133/960 (14%)

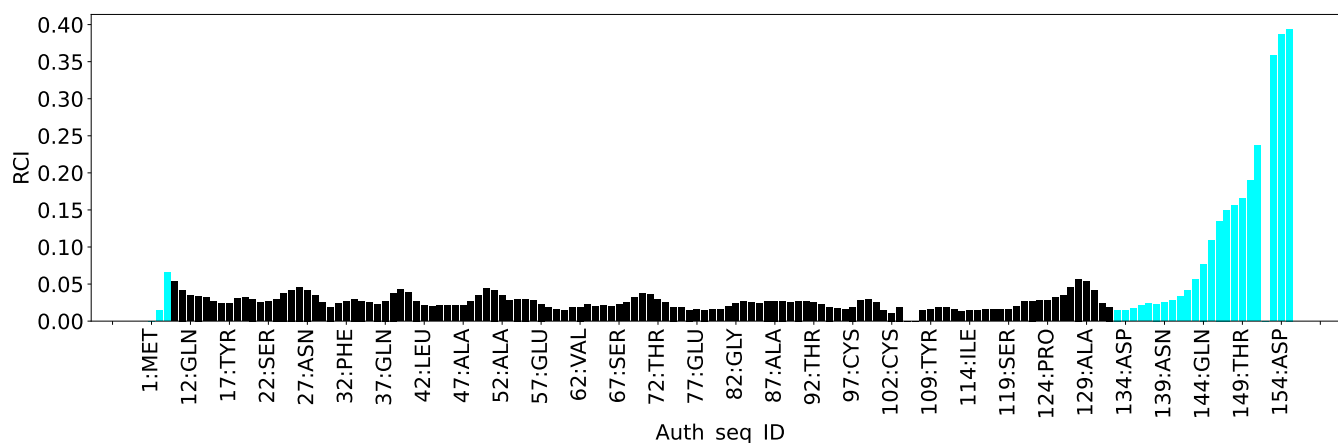
### 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain B:



## 7.3 Chemical shift list 3

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_list\_3*

### 7.3.1 Bookkeeping [i](#)

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

Total number of shifts	1044
Number of shifts mapped to atoms	1044
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	$0.27 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	126	$0.78 \pm 0.09$	Should be checked
$^{13}\text{C}'$	135	$0.26 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	132	$-1.09 \pm 0.17$	Should be applied

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 897 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	460/2467 (19%)	112/998 (11%)	236/998 (24%)	112/471 (24%)
Sidechain	372/3626 (10%)	207/2375 (9%)	165/1139 (14%)	0/112 (0%)
Aromatic	65/576 (11%)	33/280 (12%)	31/276 (11%)	1/20 (5%)
Overall	897/6669 (13%)	352/3653 (10%)	432/2413 (18%)	113/603 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 1044 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	539/3856 (14%)	132/1564 (8%)	275/1560 (18%)	132/732 (18%)
Sidechain	428/5612 (8%)	237/3656 (6%)	191/1768 (11%)	0/188 (0%)
Aromatic	77/840 (9%)	39/408 (10%)	37/392 (9%)	1/40 (2%)
Overall	1044/10308 (10%)	408/5628 (7%)	503/3720 (14%)	133/960 (14%)



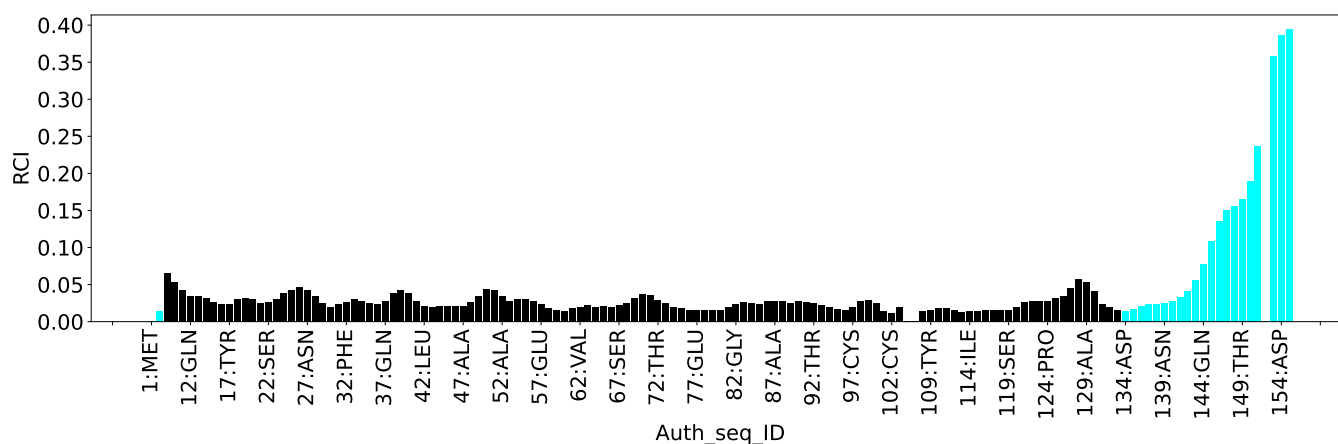
### 7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain C:



## 7.4 Chemical shift list 4

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_list\_4*

### 7.4.1 Bookkeeping [i](#)

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

Total number of shifts	1046
Number of shifts mapped to atoms	1046
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	$0.25 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	128	$0.86 \pm 0.14$	Should be checked
$^{13}\text{C}'$	137	$0.28 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	133	$-1.15 \pm 0.30$	Should be applied

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 13%, i.e. 888 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	455/2467 (18%)	111/998 (11%)	233/998 (23%)	111/471 (24%)
Sidechain	368/3626 (10%)	204/2375 (9%)	164/1139 (14%)	0/112 (0%)
Aromatic	65/576 (11%)	33/280 (12%)	31/276 (11%)	1/20 (5%)
Overall	888/6669 (13%)	348/3653 (10%)	428/2413 (18%)	112/603 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 1046 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	542/3856 (14%)	133/1564 (9%)	276/1560 (18%)	133/732 (18%)
Sidechain	427/5612 (8%)	234/3656 (6%)	193/1768 (11%)	0/188 (0%)
Aromatic	77/840 (9%)	39/408 (10%)	37/392 (9%)	1/40 (2%)
Overall	1046/10308 (10%)	406/5628 (7%)	506/3720 (14%)	134/960 (14%)

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

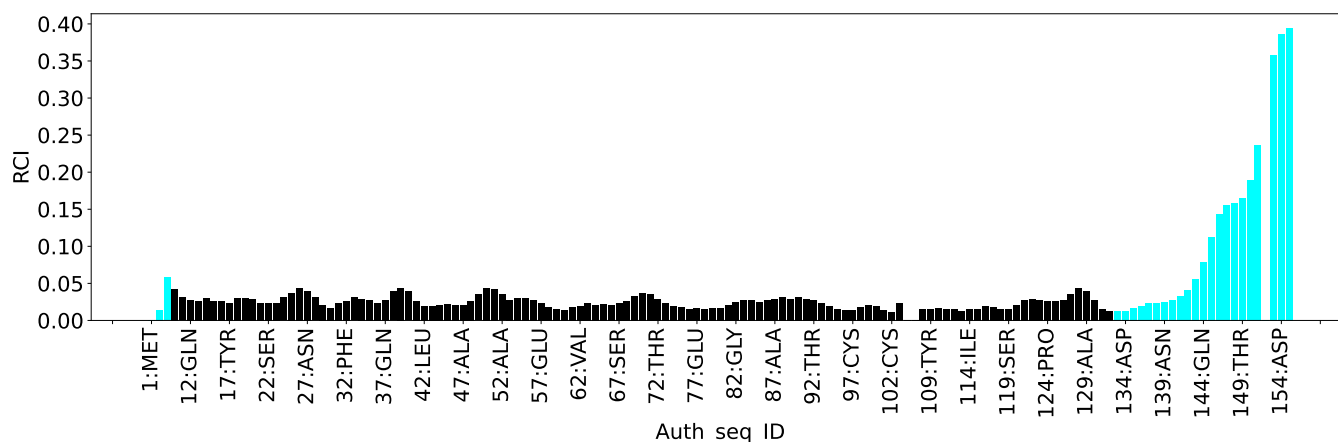
There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-

defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain D:



## 7.5 Chemical shift list 5

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_5*

### 7.5.1 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	223
Number of shifts mapped to atoms	223
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

### 7.5.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	36	$-0.32 \pm 0.21$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	33	$0.61 \pm 0.29$	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{15}\text{N}$	32	-0.40 $\pm$ 0.47	None needed ( $< 0.5$ ppm)

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/2467 (0%)	0/998 (0%)	0/998 (0%)	0/471 (0%)
Sidechain	0/3626 (0%)	0/2375 (0%)	0/1139 (0%)	0/112 (0%)
Aromatic	0/576 (0%)	0/280 (0%)	0/276 (0%)	0/20 (0%)
Overall	0/6669 (0%)	0/3653 (0%)	0/2413 (0%)	0/603 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 222 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	99/3856 (3%)	31/1564 (2%)	36/1560 (2%)	32/732 (4%)
Sidechain	113/5612 (2%)	63/3656 (2%)	50/1768 (3%)	0/188 (0%)
Aromatic	10/840 (1%)	9/408 (2%)	0/392 (0%)	1/40 (2%)
Overall	222/10308 (2%)	103/5628 (2%)	86/3720 (2%)	33/960 (3%)

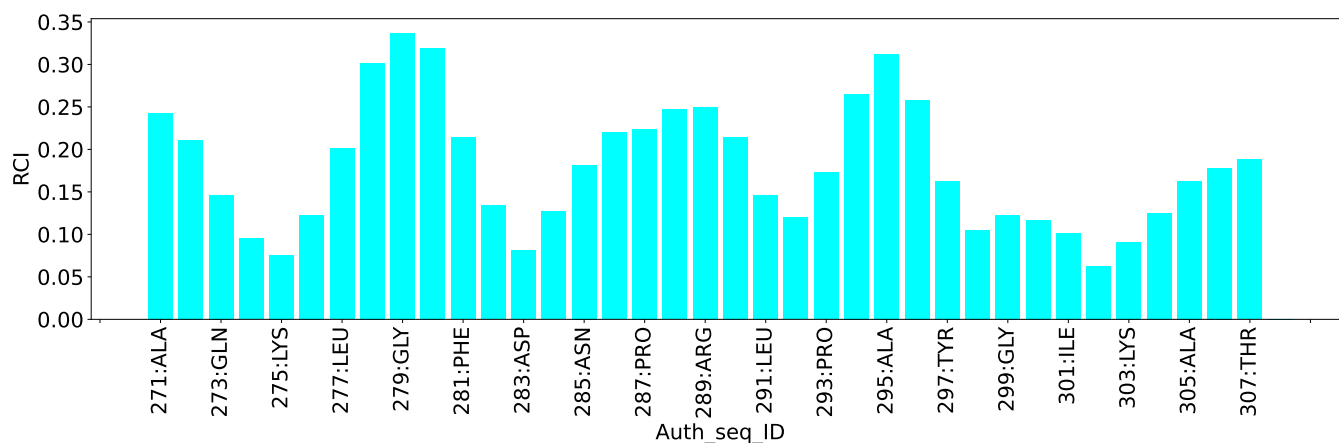
### 7.5.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain E:



## 7.6 Chemical shift list 6

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_6*

### 7.6.1 Bookkeeping [i](#)

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

Total number of shifts	223
Number of shifts mapped to atoms	223
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	36	$-0.32 \pm 0.30$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	33	$0.62 \pm 0.34$	None needed (imprecise)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	32	$-0.41 \pm 0.49$	None needed ( $< 0.5$ ppm)

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 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	0/2467 (0%)	0/998 (0%)	0/998 (0%)	0/471 (0%)
Sidechain	0/3626 (0%)	0/2375 (0%)	0/1139 (0%)	0/112 (0%)
Aromatic	0/576 (0%)	0/280 (0%)	0/276 (0%)	0/20 (0%)
Overall	0/6669 (0%)	0/3653 (0%)	0/2413 (0%)	0/603 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 222 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 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	99/3856 (3%)	31/1564 (2%)	36/1560 (2%)	32/732 (4%)
Sidechain	113/5612 (2%)	63/3656 (2%)	50/1768 (3%)	0/188 (0%)
Aromatic	10/840 (1%)	9/408 (2%)	0/392 (0%)	1/40 (2%)
Overall	222/10308 (2%)	103/5628 (2%)	86/3720 (2%)	33/960 (3%)

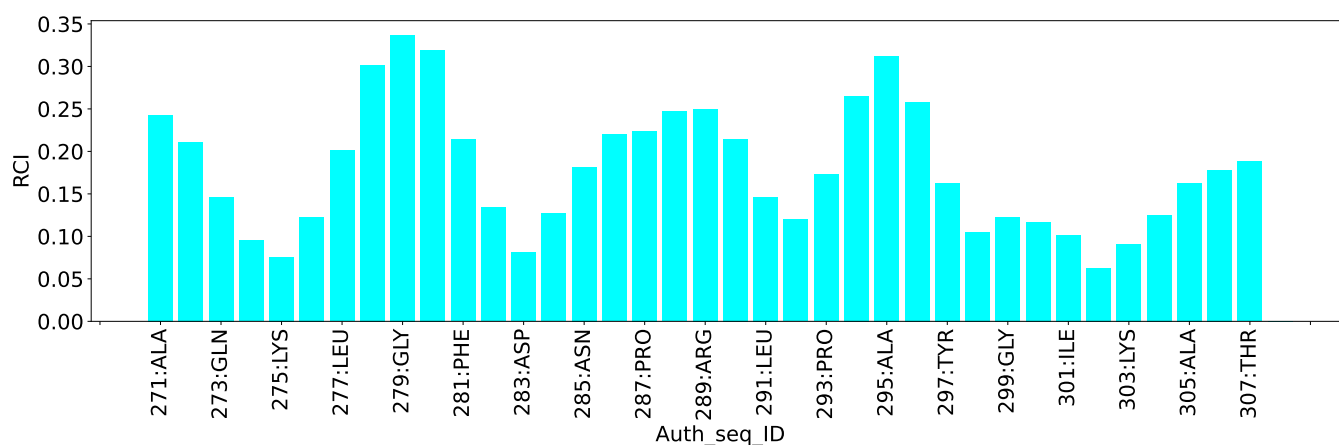
### 7.6.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain F:



## 7.7 Chemical shift list 7

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_7*

### 7.7.1 Bookkeeping [i](#)

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

Total number of shifts	223
Number of shifts mapped to atoms	223
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	36	$-0.32 \pm 0.26$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	33	$0.60 \pm 0.26$	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	32	$-0.41 \pm 0.52$	None needed ( $< 0.5$ ppm)

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 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	0/2467 (0%)	0/998 (0%)	0/998 (0%)	0/471 (0%)
Sidechain	0/3626 (0%)	0/2375 (0%)	0/1139 (0%)	0/112 (0%)
Aromatic	0/576 (0%)	0/280 (0%)	0/276 (0%)	0/20 (0%)
Overall	0/6669 (0%)	0/3653 (0%)	0/2413 (0%)	0/603 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 222 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 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	99/3856 (3%)	31/1564 (2%)	36/1560 (2%)	32/732 (4%)
Sidechain	113/5612 (2%)	63/3656 (2%)	50/1768 (3%)	0/188 (0%)
Aromatic	10/840 (1%)	9/408 (2%)	0/392 (0%)	1/40 (2%)
Overall	222/10308 (2%)	103/5628 (2%)	86/3720 (2%)	33/960 (3%)

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

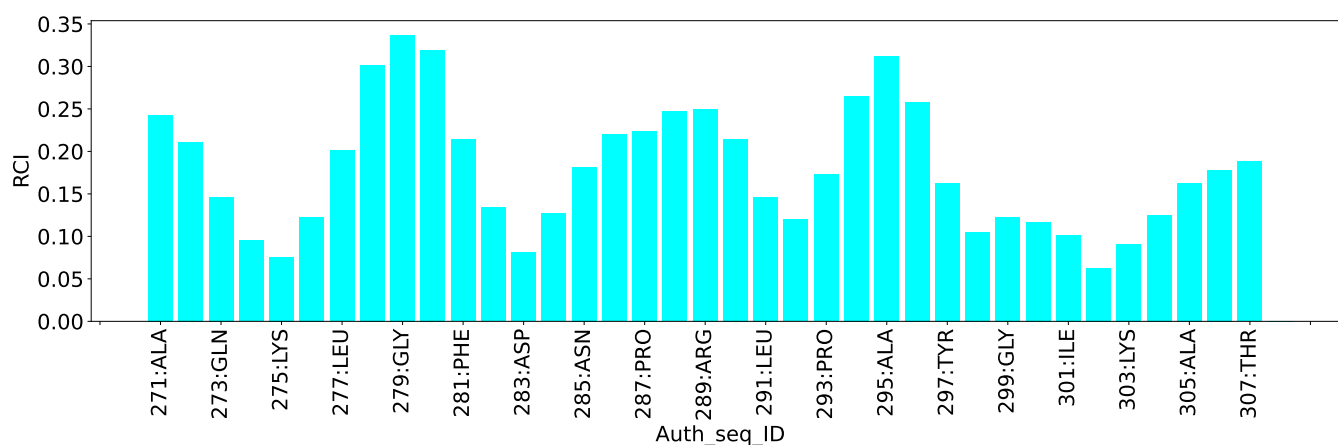
There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain G:





## 7.8 Chemical shift list 8

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shift\_8*

### 7.8.1 Bookkeeping [i](#)

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

Total number of shifts	223
Number of shifts mapped to atoms	223
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	36	$-0.33 \pm 0.32$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	33	$0.60 \pm 0.39$	None needed (imprecise)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	32	$-0.41 \pm 0.54$	None needed ( $< 0.5$ ppm)

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 6669. 0 out of 80 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	0/2467 (0%)	0/998 (0%)	0/998 (0%)	0/471 (0%)
Sidechain	0/3626 (0%)	0/2375 (0%)	0/1139 (0%)	0/112 (0%)
Aromatic	0/576 (0%)	0/280 (0%)	0/276 (0%)	0/20 (0%)
Overall	0/6669 (0%)	0/3653 (0%)	0/2413 (0%)	0/603 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 222 atoms were assigned a chemical shift out of a possible 10308. 0 out of 112 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	99/3856 (3%)	31/1564 (2%)	36/1560 (2%)	32/732 (4%)
Sidechain	113/5612 (2%)	63/3656 (2%)	50/1768 (3%)	0/188 (0%)
Aromatic	10/840 (1%)	9/408 (2%)	0/392 (0%)	1/40 (2%)
Overall	222/10308 (2%)	103/5628 (2%)	86/3720 (2%)	33/960 (3%)

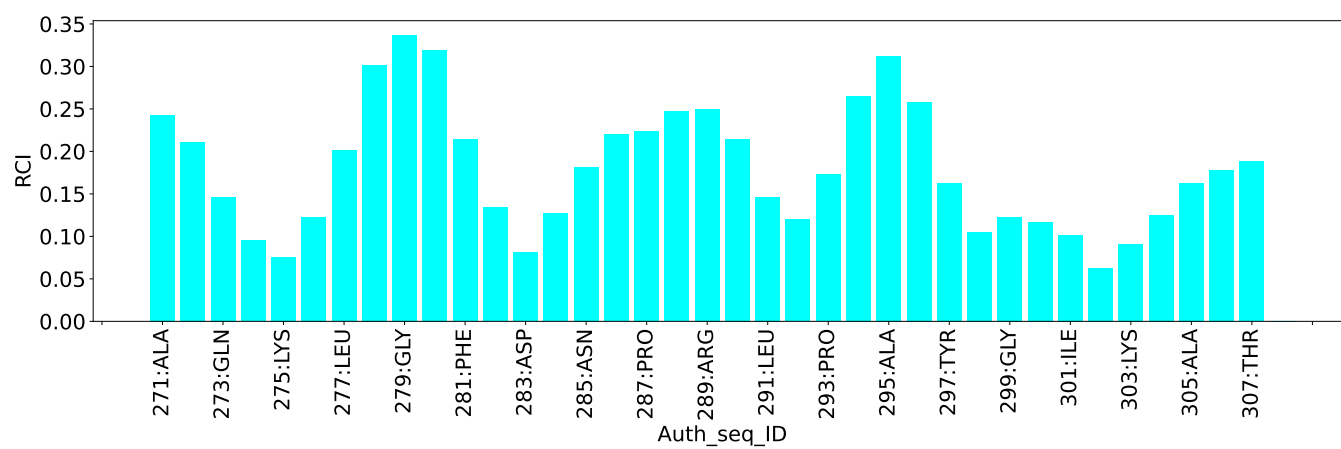
### 7.8.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain H:



## 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	1710
Intra-residue ( $ i-j =0$ )	0
Sequential ( $ i-j =1$ )	673
Medium range ( $ i-j >1$ and $ i-j <5$ )	360
Long range ( $ i-j \geq 5$ )	428
Inter-chain	245
Hydrogen bond restraints	4
Disulfide bond restraints	0
Total dihedral-angle restraints	1012
Number of unmapped restraints	0
Number of restraints per residue	3.5
Number of long range restraints per residue <sup>1</sup>	0.5

<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)	67.9	0.2
0.2-0.5 (Medium)	80.5	0.5
>0.5 (Large)	65.6	5.82

### 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)	108.2	9.86
10.0-20.0 (Medium)	0.3	11.97
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

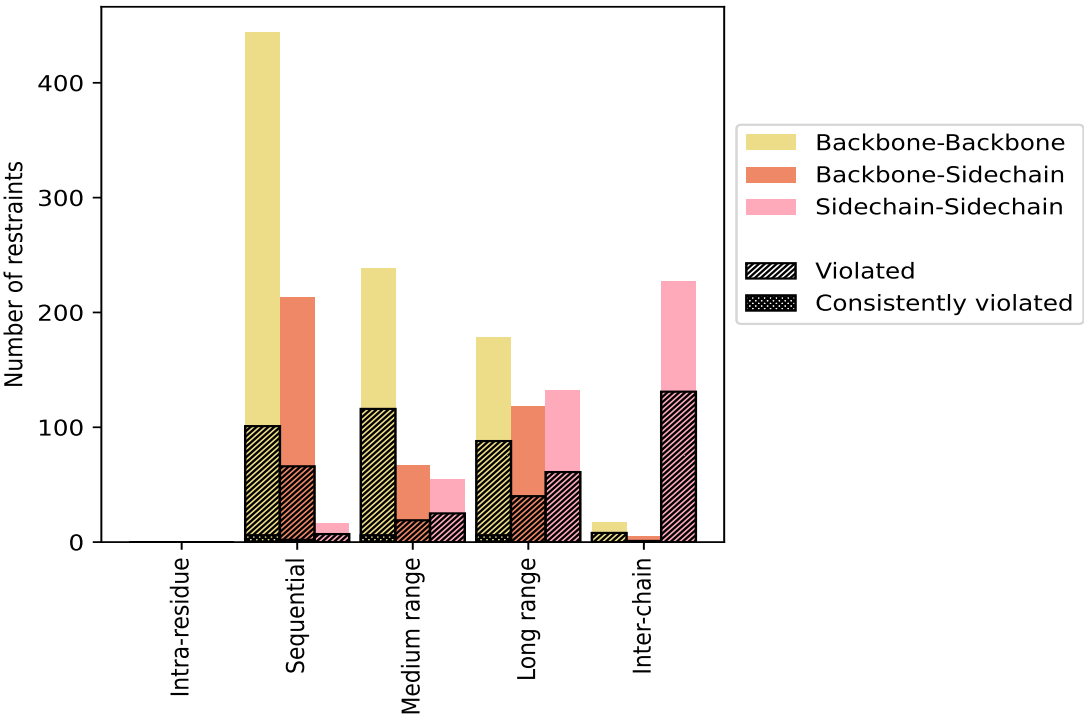
### 9.1 Summary of distance violations ⓘ

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>	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	673	39.4	174	25.9	10.2	8	1.2	0.5
Backbone-Backbone	444	26.0	101	22.7	5.9	6	1.4	0.4
Backbone-Sidechain	213	12.5	66	31.0	3.9	2	0.9	0.1
Sidechain-Sidechain	16	0.9	7	43.8	0.4	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	360	21.1	160	44.4	9.4	6	1.7	0.4
Backbone-Backbone	238	13.9	116	48.7	6.8	6	2.5	0.4
Backbone-Sidechain	67	3.9	19	28.4	1.1	0	0.0	0.0
Sidechain-Sidechain	55	3.2	25	45.5	1.5	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	428	25.0	189	44.2	11.1	6	1.4	0.4
Backbone-Backbone	178	10.4	88	49.4	5.1	6	3.4	0.4
Backbone-Sidechain	118	6.9	40	33.9	2.3	0	0.0	0.0
Sidechain-Sidechain	132	7.7	61	46.2	3.6	0	0.0	0.0
<a href="#">Inter-chain</a>	245	14.3	136	55.5	8.0	0	0.0	0.0
Backbone-Backbone	17	1.0	8	47.1	0.5	0	0.0	0.0
Backbone-Sidechain	5	0.3	1	20.0	0.1	0	0.0	0.0
Sidechain-Sidechain	223	13.0	127	57.0	7.4	0	0.0	0.0
<a href="#">Hydrogen bond</a>	4	0.2	4	100.0	0.2	0	0.0	0.0
<a href="#">Disulfide bond</a>	0	0.0	0	0.0	0.0	0	0.0	0.0
<a href="#">Total</a>	1710	100.0	663	38.8	38.8	20	1.2	1.2
Backbone-Backbone	877	51.3	313	35.7	18.3	18	2.1	1.1
Backbone-Sidechain	403	23.6	126	31.3	7.4	2	0.5	0.1
Sidechain-Sidechain	430	25.1	224	52.1	13.1	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	69	60	66	31	226	0.44	3.73	0.46	0.26
2	0	71	60	57	24	212	0.57	4.27	0.66	0.32
3	0	73	63	74	21	231	0.52	3.48	0.54	0.3
4	0	77	45	55	21	198	0.49	4.13	0.53	0.29
5	0	74	50	61	32	217	0.43	2.42	0.39	0.31
6	0	77	65	70	31	243	0.61	5.82	0.8	0.27
7	0	71	55	71	23	220	0.51	3.21	0.56	0.29
8	0	65	58	63	33	219	0.44	2.43	0.43	0.27
9	0	76	62	54	26	218	0.47	3.27	0.49	0.29
10	0	70	55	67	17	209	0.46	3.06	0.45	0.29

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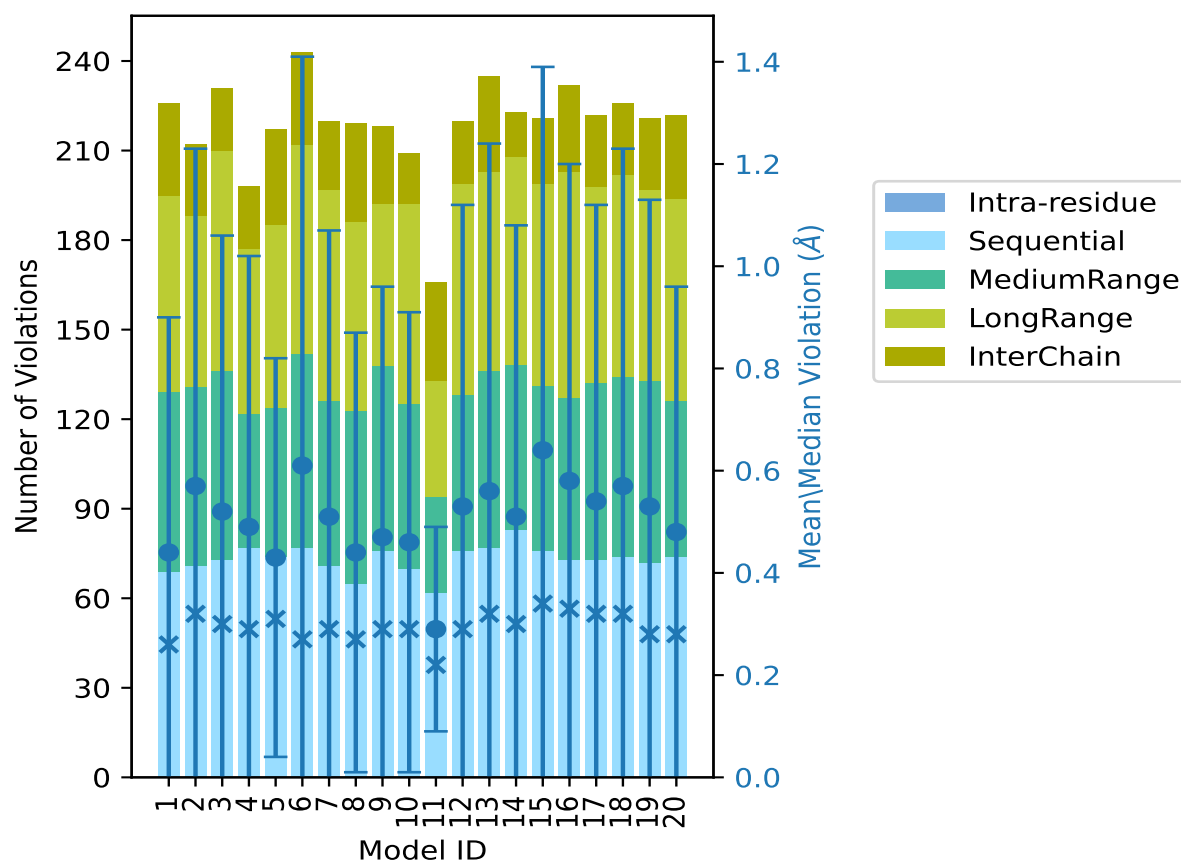
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	0	62	32	39	33	166	0.29	1.29	0.2	0.22
12	0	76	52	71	21	220	0.53	3.4	0.59	0.29
13	0	77	59	67	32	235	0.56	5.68	0.68	0.32
14	0	83	55	70	15	223	0.51	3.75	0.57	0.3
15	0	76	55	68	22	221	0.64	4.48	0.75	0.34
16	0	73	54	76	29	232	0.58	3.32	0.62	0.33
17	0	73	59	66	24	222	0.54	3.8	0.58	0.32
18	0	74	60	68	24	226	0.57	5.38	0.66	0.32
19	0	72	61	64	24	221	0.53	3.73	0.6	0.28
20	0	74	52	68	28	222	0.48	3.02	0.48	0.28

<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

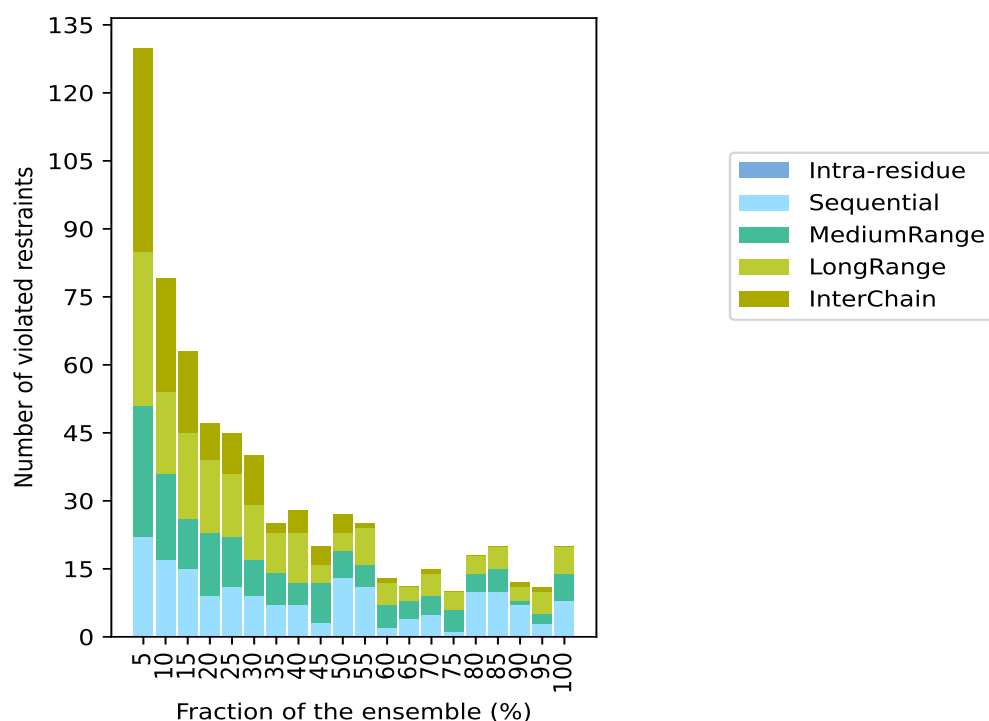
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1047(IR:0, SQ:499, MR:200, LR:239, IC:109) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	22	29	34	45	130	1	5.0
0	17	19	18	25	79	2	10.0
0	15	11	19	18	63	3	15.0
0	9	14	16	8	47	4	20.0
0	11	11	14	9	45	5	25.0
0	9	8	12	11	40	6	30.0
0	7	7	9	2	25	7	35.0
0	7	5	11	5	28	8	40.0
0	3	9	4	4	20	9	45.0
0	13	6	4	4	27	10	50.0
0	11	5	8	1	25	11	55.0
0	2	5	5	1	13	12	60.0
0	4	4	3	0	11	13	65.0
0	5	4	5	1	15	14	70.0
0	1	5	4	0	10	15	75.0
0	10	4	4	0	18	16	80.0
0	10	5	5	0	20	17	85.0
0	7	1	3	1	12	18	90.0
0	3	2	5	1	11	19	95.0
0	8	6	6	0	20	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

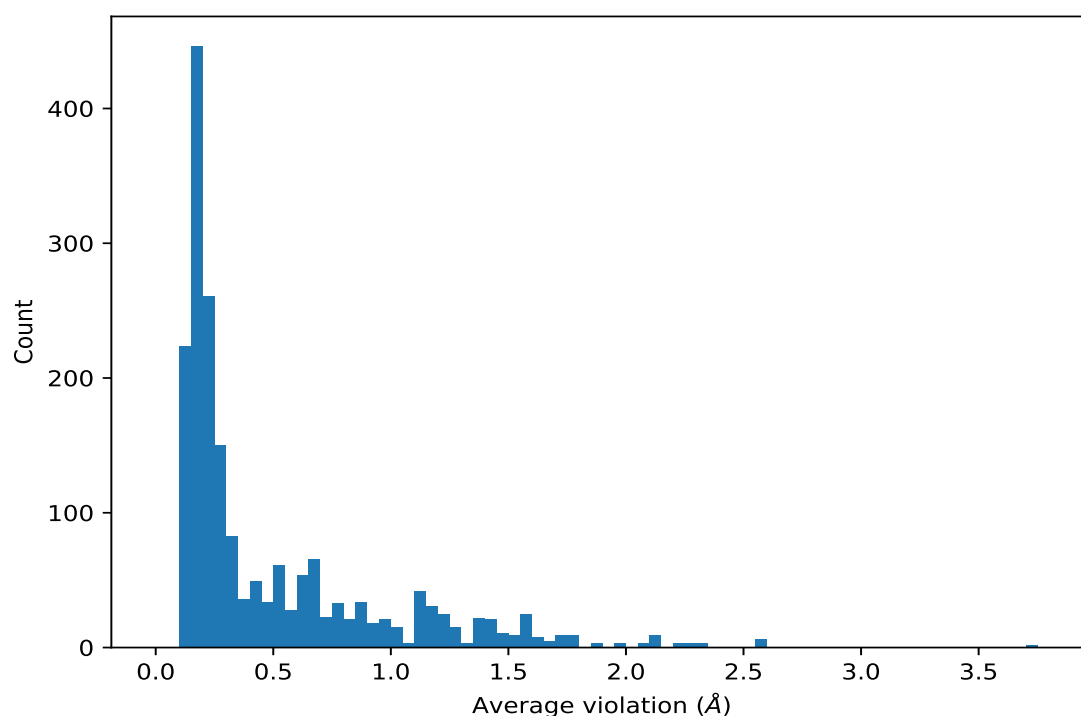
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	20	1.58	0.36	1.54
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	20	0.94	0.24	0.9
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	20	0.92	0.16	0.95
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	20	0.91	0.12	0.91
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	20	0.84	0.21	0.82
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	20	0.74	0.13	0.78
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	20	0.54	0.14	0.54
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	20	0.54	0.11	0.52
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	20	0.54	0.12	0.56
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	20	0.54	0.12	0.56
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	20	0.52	0.19	0.55
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	20	0.48	0.16	0.5
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	20	0.43	0.05	0.44
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	20	0.43	0.1	0.44
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	20	0.43	0.1	0.44
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	20	0.4	0.16	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	20	0.36	0.14	0.36
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	20	0.34	0.09	0.34
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	20	0.34	0.09	0.34
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	20	0.29	0.07	0.32
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	20	0.29	0.06	0.29
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	20	0.26	0.12	0.24
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	19	1.26	0.57	1.24
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	19	1.26	0.57	1.24
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	19	1.26	0.57	1.24
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	19	0.93	0.03	0.93
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	19	0.93	0.03	0.93
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	19	0.93	0.03	0.93
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	19	0.61	0.23	0.64
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	19	0.5	0.24	0.5
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	19	0.41	0.12	0.38
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	19	0.36	0.14	0.36
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	19	0.34	0.14	0.33
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	19	0.34	0.08	0.34
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	19	0.27	0.13	0.24
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	19	0.27	0.13	0.24
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	19	0.27	0.13	0.24
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	19	0.21	0.06	0.21
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	19	0.17	0.03	0.17
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	18	1.44	0.25	1.4
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	18	1.44	0.25	1.4
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	18	1.44	0.25	1.4
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	18	0.68	0.06	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	18	0.68	0.06	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	18	0.68	0.06	0.67
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	18	0.59	0.07	0.6
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	18	0.59	0.07	0.6
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	18	0.59	0.07	0.6
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	18	0.5	0.22	0.48
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	18	0.5	0.22	0.48
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	18	0.5	0.22	0.48
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	18	0.44	0.22	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	18	0.44	0.22	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	18	0.44	0.22	0.47
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	18	0.44	0.16	0.48
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	18	0.44	0.16	0.48
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	18	0.35	0.12	0.35
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	18	0.31	0.15	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	18	0.29	0.07	0.29
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	18	0.27	0.08	0.29
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	18	0.22	0.09	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	18	0.22	0.09	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	18	0.22	0.09	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	18	0.22	0.09	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	18	0.22	0.09	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	18	0.22	0.09	0.2
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	18	0.16	0.04	0.15
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	17	1.59	0.81	1.68
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	17	1.59	0.81	1.68
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	17	1.59	0.81	1.68
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	17	1.24	0.38	1.25
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	17	1.24	0.38	1.25
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	17	1.24	0.38	1.25
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	17	1.12	0.37	1.02
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	17	1.12	0.37	1.02
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	17	1.12	0.37	1.02
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	17	0.69	0.2	0.75
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	17	0.69	0.2	0.75
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	17	0.69	0.2	0.75
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	17	0.53	0.23	0.59
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	17	0.46	0.2	0.44
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	17	0.46	0.2	0.44
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	17	0.46	0.2	0.44
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	17	0.44	0.23	0.35
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	17	0.41	0.2	0.39
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	17	0.41	0.19	0.4
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	17	0.41	0.17	0.4
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	17	0.36	0.16	0.35
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	17	0.36	0.16	0.35
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	17	0.35	0.15	0.37
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	17	0.3	0.09	0.3
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	17	0.23	0.06	0.24
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	17	0.23	0.06	0.23
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	17	0.22	0.04	0.22
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	17	0.22	0.04	0.23
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	17	0.22	0.04	0.23
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	17	0.22	0.04	0.23
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	17	0.21	0.06	0.19
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	17	0.2	0.08	0.19
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	17	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	16	2.56	1.15	3.06
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	16	2.56	1.15	3.06
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	16	2.56	1.15	3.06
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	16	2.56	1.15	3.06
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	16	2.56	1.15	3.06
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	16	2.56	1.15	3.06
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	16	1.11	0.38	1.13
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	16	1.11	0.38	1.13
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	16	1.11	0.38	1.13
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	16	0.77	0.26	0.82
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	16	0.77	0.26	0.82
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	16	0.77	0.26	0.82
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	16	0.55	0.41	0.4
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	16	0.53	0.22	0.56
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	16	0.52	0.17	0.53
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	16	0.44	0.23	0.43
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	16	0.37	0.17	0.33
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	16	0.37	0.17	0.33
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	16	0.36	0.18	0.28
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	16	0.31	0.18	0.29
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	16	0.29	0.15	0.24
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	16	0.27	0.13	0.22
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	16	0.24	0.07	0.26
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	16	0.22	0.08	0.2
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	16	0.2	0.05	0.2
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	16	0.19	0.05	0.18
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	16	0.14	0.04	0.14
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	16	0.14	0.03	0.14
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	15	2.12	1.36	2.4
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	15	2.12	1.36	2.4
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	15	1.4	0.67	1.21
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	15	1.4	0.67	1.21
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	15	1.4	0.67	1.21
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	15	1.4	0.67	1.21
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	15	1.4	0.67	1.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	15	1.4	0.67	1.21
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	15	1.4	0.67	1.21
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	15	1.4	0.67	1.21
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	15	1.4	0.67	1.21
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	15	0.4	0.24	0.36
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	15	0.32	0.14	0.32
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	15	0.32	0.14	0.32
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	15	0.31	0.14	0.29
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	15	0.3	0.11	0.31
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	15	0.29	0.11	0.26
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	15	0.25	0.07	0.26
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	15	0.24	0.1	0.24
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	15	0.21	0.09	0.18
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	14	2.25	1.95	1.67
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	14	2.25	1.95	1.67
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	14	2.25	1.95	1.67
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	14	1.78	0.29	1.78
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	14	1.78	0.29	1.78
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	14	1.78	0.29	1.78
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	14	1.78	0.63	2.0
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	14	1.78	0.63	2.0
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	14	1.78	0.63	2.0
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	14	1.78	0.63	2.0
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	14	1.78	0.63	2.0
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	14	1.78	0.63	2.0
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	14	1.48	0.64	1.74
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	14	1.48	0.64	1.74
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	14	1.48	0.64	1.74
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	14	1.35	0.75	1.27
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	14	1.35	0.75	1.27
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	14	1.29	0.73	1.04
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	14	1.29	0.73	1.04
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	14	1.29	0.73	1.04
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	14	0.45	0.33	0.31
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	14	0.32	0.18	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	14	0.29	0.06	0.26
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	14	0.28	0.1	0.29
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	14	0.27	0.11	0.25
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	14	0.27	0.11	0.25
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	14	0.27	0.11	0.25
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	14	0.27	0.11	0.25
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	14	0.27	0.11	0.25
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	14	0.27	0.11	0.25
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	14	0.25	0.1	0.26
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	14	0.24	0.1	0.2
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	14	0.16	0.05	0.15
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	14	0.14	0.03	0.15
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	13	1.67	0.65	1.84
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	13	1.4	1.29	1.18
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	13	1.4	1.29	1.18
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	13	1.37	0.66	1.12
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	13	0.73	0.53	0.52
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	13	0.73	0.53	0.52
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	13	0.73	0.53	0.52
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	13	0.73	0.53	0.52
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	13	0.73	0.53	0.52
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	13	0.73	0.53	0.52
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	13	0.43	0.23	0.38
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	13	0.41	0.16	0.44
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	13	0.28	0.08	0.3
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	13	0.28	0.08	0.3
(1,640)	1:92:B:THR:H	1:94:B:MET:H	13	0.27	0.13	0.27
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	13	0.26	0.11	0.27
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	13	0.25	0.13	0.2
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	13	0.22	0.09	0.17
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	12	1.49	0.81	1.57
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	12	1.49	0.81	1.57
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	12	1.49	0.81	1.57
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	12	1.21	0.45	1.17
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	12	1.21	0.45	1.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	12	1.21	0.45	1.17
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	12	1.21	0.45	1.17
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	12	1.21	0.45	1.17
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	12	1.21	0.45	1.17
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	12	1.21	0.45	1.17
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	12	1.21	0.45	1.17
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	12	1.21	0.45	1.17
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	12	1.15	0.41	1.3
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	12	1.01	0.65	1.1
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	12	1.01	0.65	1.1
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	12	1.01	0.65	1.1
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	12	0.95	0.61	0.77
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	12	0.95	0.61	0.77
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	12	0.95	0.61	0.77
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	12	0.9	0.37	0.88
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	12	0.9	0.37	0.88
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	12	0.85	0.35	0.93
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	12	0.85	0.35	0.93
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	12	0.74	0.17	0.78
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	12	0.33	0.17	0.28
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	12	0.33	0.17	0.28
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	12	0.22	0.06	0.24
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	12	0.22	0.06	0.24
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	12	0.22	0.06	0.24
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	12	0.22	0.06	0.24
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	12	0.22	0.06	0.24
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	12	0.22	0.06	0.24
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	12	0.22	0.06	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	12	0.18	0.05	0.16
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	12	0.17	0.03	0.16
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	11	1.69	0.65	1.63
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	11	1.69	0.65	1.63
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	11	1.69	0.65	1.63
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	11	1.6	0.82	1.6
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	11	1.6	0.82	1.6
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	11	1.6	0.82	1.6
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	11	1.57	0.97	0.98
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	11	1.57	0.97	0.98
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	11	1.57	0.97	0.98
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	11	1.32	0.74	0.87
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	11	1.32	0.74	0.87
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	11	1.32	0.74	0.87
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	11	1.2	0.63	1.25
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	11	1.2	0.63	1.25
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	11	1.2	0.63	1.25
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	11	1.19	0.38	1.21
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	11	1.19	0.38	1.21
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	11	1.11	0.52	1.2
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	11	1.11	0.52	1.2
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	11	1.11	0.52	1.2
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	11	0.92	0.54	0.82
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	11	0.92	0.54	0.82
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	11	0.92	0.54	0.82
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	11	0.86	0.92	0.31
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	11	0.86	0.92	0.31
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	11	0.86	0.92	0.31
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	11	0.78	0.29	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	11	0.78	0.29	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	11	0.78	0.29	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	11	0.78	0.29	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	11	0.78	0.29	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	11	0.78	0.29	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	11	0.78	0.29	0.72

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	11	0.78	0.29	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	11	0.78	0.29	0.72
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	11	0.58	0.2	0.67
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	11	0.58	0.2	0.67
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	11	0.58	0.2	0.67
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	11	0.52	0.3	0.5
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	11	0.52	0.3	0.5
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	11	0.52	0.2	0.6
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	11	0.52	0.2	0.6
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	11	0.52	0.2	0.6
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	11	0.48	0.12	0.5
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	11	0.48	0.12	0.5
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	11	0.44	0.53	0.22
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	11	0.44	0.53	0.22
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	11	0.44	0.53	0.22
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	11	0.34	0.2	0.31
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	11	0.28	0.08	0.3
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	11	0.26	0.08	0.26
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	11	0.26	0.11	0.23
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	11	0.2	0.05	0.22
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	11	0.2	0.06	0.2
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	11	0.2	0.07	0.19
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	11	0.19	0.06	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	11	0.19	0.06	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	11	0.19	0.06	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	11	0.19	0.06	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	11	0.19	0.06	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	11	0.19	0.06	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	11	0.19	0.06	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	11	0.19	0.06	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	11	0.19	0.06	0.16
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	11	0.16	0.03	0.16
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	11	0.15	0.04	0.14
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	11	0.15	0.04	0.14
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	10	1.71	1.21	1.52
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	10	1.71	1.21	1.52
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	10	1.46	0.65	1.59
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	10	1.46	0.65	1.59
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	10	1.46	0.65	1.59
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	10	1.22	0.79	1.08
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	10	1.22	0.79	1.08
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	10	1.16	0.67	0.9
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	10	1.16	0.67	0.9
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	10	1.15	0.51	1.03
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	10	1.15	0.51	1.03
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	10	1.15	0.51	1.03
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	10	1.1	0.57	0.88
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	10	1.1	0.57	0.88
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	10	1.1	0.57	0.88

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	10	1.1	0.57	0.88
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	10	1.1	0.57	0.88
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	10	1.1	0.57	0.88
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	10	1.1	0.57	0.88
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	10	1.1	0.57	0.88
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	10	1.1	0.57	0.88
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	10	0.98	0.79	0.55
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	10	0.98	0.79	0.55
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	10	0.98	0.79	0.55
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	10	0.98	0.47	0.9
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	10	0.98	0.47	0.9
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	10	0.82	0.48	0.7
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	10	0.82	0.5	0.89
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	10	0.67	0.27	0.76
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	10	0.67	0.27	0.76
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	10	0.57	0.41	0.45
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	10	0.54	0.26	0.49
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	10	0.54	0.26	0.49
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	10	0.54	0.26	0.49
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	10	0.54	0.26	0.49
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	10	0.46	0.19	0.46
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	10	0.45	0.39	0.36
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	10	0.45	0.39	0.36
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	10	0.42	0.19	0.38
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	10	0.42	0.19	0.38
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	10	0.34	0.08	0.34
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	10	0.34	0.08	0.34
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	10	0.34	0.08	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	10	0.34	0.08	0.34
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	10	0.34	0.08	0.34
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	10	0.34	0.08	0.34
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	10	0.29	0.15	0.26
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	10	0.26	0.09	0.29
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	10	0.26	0.1	0.22
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	10	0.24	0.17	0.18
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	10	0.21	0.06	0.22
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	10	0.2	0.05	0.2
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	10	0.18	0.07	0.16
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	10	0.18	0.07	0.16
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	10	0.18	0.07	0.16
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	10	0.18	0.05	0.19
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	10	0.18	0.05	0.19
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	10	0.18	0.05	0.19
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	10	0.17	0.06	0.15
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	10	0.15	0.04	0.14
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	9	1.19	0.58	1.17
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	9	1.19	0.58	1.17
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	9	0.77	0.48	0.67
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	9	0.77	0.48	0.67
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	9	0.77	0.48	0.67
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	9	0.66	0.32	0.61
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	9	0.66	0.32	0.61
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	9	0.66	0.32	0.61
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	9	0.62	0.42	0.54
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	9	0.6	0.29	0.59
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	9	0.6	0.29	0.59
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	9	0.6	0.29	0.59
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	9	0.48	0.19	0.48
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	9	0.48	0.19	0.48
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	9	0.48	0.19	0.48
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	9	0.43	0.31	0.29
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	9	0.3	0.18	0.26
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	9	0.29	0.14	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	9	0.25	0.12	0.18
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	9	0.25	0.08	0.26
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	9	0.24	0.08	0.26
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	9	0.24	0.07	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	9	0.24	0.07	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	9	0.24	0.07	0.22
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	9	0.23	0.1	0.23
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	9	0.23	0.09	0.23
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	9	0.2	0.08	0.17
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	9	0.18	0.07	0.17
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	9	0.18	0.07	0.17
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	9	0.16	0.04	0.15
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	9	0.16	0.04	0.15
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	9	0.16	0.04	0.16
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	9	0.13	0.03	0.12
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	8	1.68	1.16	1.72
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	8	0.83	0.7	0.57
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	8	0.83	0.7	0.57
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	8	0.82	0.49	0.64
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	8	0.82	0.49	0.64
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	8	0.82	0.49	0.64

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	8	0.82	0.49	0.64
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	8	0.82	0.49	0.64
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	8	0.82	0.49	0.64
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	8	0.82	0.49	0.64
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	8	0.82	0.49	0.64
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	8	0.82	0.49	0.64
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	8	0.73	0.22	0.7
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	8	0.73	0.22	0.7
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	8	0.73	0.22	0.7
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	8	0.73	0.22	0.7
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	8	0.73	0.22	0.7
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	8	0.73	0.22	0.7
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	8	0.67	0.3	0.76
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	8	0.67	0.3	0.76
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	8	0.67	0.3	0.76
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	8	0.67	0.3	0.76
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	8	0.67	0.3	0.76
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	8	0.67	0.3	0.76
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	8	0.66	0.34	0.67
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	8	0.66	0.34	0.67
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	8	0.66	0.34	0.67
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	8	0.53	0.22	0.5
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	8	0.53	0.22	0.5
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	8	0.53	0.22	0.5
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	8	0.41	0.11	0.44
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	8	0.39	0.11	0.36
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	8	0.32	0.13	0.3
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	8	0.32	0.13	0.3
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	8	0.32	0.13	0.3
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	8	0.31	0.09	0.29
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	8	0.3	0.16	0.22
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	8	0.3	0.16	0.22
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	8	0.3	0.08	0.29
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	8	0.26	0.09	0.27
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	8	0.25	0.08	0.26
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	8	0.25	0.08	0.26
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	8	0.25	0.08	0.26
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	8	0.22	0.1	0.16
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	8	0.22	0.09	0.21
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	8	0.22	0.09	0.21
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	8	0.22	0.09	0.21
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	8	0.22	0.09	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	8	0.22	0.09	0.21
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	8	0.22	0.09	0.21
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	8	0.21	0.04	0.2
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	8	0.2	0.08	0.2
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	8	0.18	0.08	0.16
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	8	0.18	0.08	0.16
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	8	0.17	0.05	0.16
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	8	0.17	0.05	0.16
(1,360)	1:122:A:THR:H	1:18:B:THR:H	8	0.16	0.06	0.15
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	8	0.16	0.03	0.16
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	8	0.16	0.03	0.15
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	8	0.16	0.03	0.15
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	8	0.16	0.03	0.15
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	8	0.15	0.04	0.15
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	8	0.15	0.04	0.15
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	8	0.15	0.04	0.15
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	8	0.15	0.04	0.15
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	8	0.15	0.04	0.15
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	8	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	8	0.15	0.04	0.14
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	8	0.15	0.01	0.15
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	8	0.14	0.04	0.14
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	7	2.22	1.04	1.61
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	7	2.22	1.04	1.61
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	7	2.22	1.04	1.61
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	7	1.98	1.45	1.07
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	7	1.98	1.45	1.07
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	7	1.98	1.45	1.07
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	7	1.51	0.24	1.49
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	7	1.51	0.24	1.49
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	7	1.51	0.24	1.49
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	7	1.02	0.5	0.99
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	7	1.02	0.5	0.99
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	7	0.71	0.41	0.47
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	7	0.71	0.41	0.47
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	7	0.64	0.27	0.7
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	7	0.64	0.27	0.7
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	7	0.64	0.27	0.7
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	7	0.62	0.47	0.36
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	7	0.43	0.15	0.49
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	7	0.43	0.15	0.49
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	7	0.43	0.15	0.49
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	7	0.39	0.15	0.31
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	7	0.36	0.18	0.27
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	7	0.31	0.11	0.3
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	7	0.3	0.04	0.31
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	7	0.29	0.11	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	7	0.27	0.16	0.21
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	7	0.27	0.1	0.29
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	7	0.22	0.09	0.17
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	7	0.22	0.1	0.2
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	7	0.19	0.08	0.15
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	7	0.18	0.03	0.16
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	7	0.18	0.05	0.18
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	7	0.18	0.05	0.18
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	7	0.16	0.03	0.15
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	7	0.16	0.03	0.15
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	7	0.16	0.03	0.15
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	7	0.16	0.06	0.12
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	7	0.16	0.06	0.12
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	7	0.16	0.06	0.12
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	7	0.16	0.06	0.12
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	7	0.16	0.06	0.12
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	7	0.16	0.06	0.12
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	7	0.15	0.04	0.13
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	7	0.14	0.03	0.15
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	7	0.13	0.03	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	7	0.13	0.03	0.11
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	7	0.12	0.02	0.11
(1,566)	1:60:B:LEU:HD11	1:61:B:ARG:H	6	1.89	0.14	1.84
(1,566)	1:60:B:LEU:HD12	1:61:B:ARG:H	6	1.89	0.14	1.84
(1,566)	1:60:B:LEU:HD13	1:61:B:ARG:H	6	1.89	0.14	1.84
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD11	6	1.64	0.34	1.54
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD12	6	1.64	0.34	1.54
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD13	6	1.64	0.34	1.54

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE1	6	1.61	1.39	1.52
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE2	6	1.61	1.39	1.52
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE1	6	1.58	0.98	1.42
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE2	6	1.58	0.98	1.42
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE3	6	1.58	0.98	1.42
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE1	6	1.58	0.98	1.42
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE2	6	1.58	0.98	1.42
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE3	6	1.58	0.98	1.42
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	6	1.27	0.77	1.09
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	6	1.27	0.77	1.09
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD11	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD12	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD13	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD11	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD12	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD13	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD11	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD12	6	1.12	0.63	1.23
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD13	6	1.12	0.63	1.23
(1,467)	1:33:B:GLN:H	1:35:B:ASP:H	6	0.88	0.53	0.84
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD1	6	0.64	0.44	0.61
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD2	6	0.64	0.44	0.61
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG21	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG22	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG23	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG21	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG22	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG23	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG21	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG22	6	0.63	0.27	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG23	6	0.63	0.27	0.67
(1,403)	1:9:B:MET:HE1	1:10:B:THR:H	6	0.6	0.18	0.71
(1,403)	1:9:B:MET:HE2	1:10:B:THR:H	6	0.6	0.18	0.71
(1,403)	1:9:B:MET:HE3	1:10:B:THR:H	6	0.6	0.18	0.71
(1,1130)	1:140:C:TYR:HD1	1:141:C:LEU:H	6	0.56	0.38	0.41

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1130)	1:140:C:TYR:HD2	1:141:C:LEU:H	6	0.56	0.38	0.41
(1,368)	1:128:A:LEU:HD11	1:129:A:ALA:H	6	0.56	0.47	0.38
(1,368)	1:128:A:LEU:HD12	1:129:A:ALA:H	6	0.56	0.47	0.38
(1,368)	1:128:A:LEU:HD13	1:129:A:ALA:H	6	0.56	0.47	0.38
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG21	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG22	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG23	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG21	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG22	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG23	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG21	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG22	6	0.53	0.32	0.4
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG23	6	0.53	0.32	0.4
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG11	6	0.39	0.13	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG12	6	0.39	0.13	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG13	6	0.39	0.13	0.38
(1,768)	1:14:C:GLN:H	1:85:C:SER:H	6	0.36	0.19	0.36
(1,120)	1:43:A:ASP:H	1:65:A:THR:H	6	0.34	0.15	0.34
(1,630)	1:87:B:ALA:H	1:89:B:ILE:H	6	0.3	0.17	0.26
(1,706)	1:118:B:VAL:HG11	1:126:B:LEU:H	6	0.29	0.11	0.23
(1,706)	1:118:B:VAL:HG12	1:126:B:LEU:H	6	0.29	0.11	0.23
(1,706)	1:118:B:VAL:HG13	1:126:B:LEU:H	6	0.29	0.11	0.23
(1,875)	1:45:C:ASP:H	1:61:C:ARG:H	6	0.27	0.09	0.28
(1,843)	1:39:C:GLU:H	1:40:C:VAL:H	6	0.27	0.08	0.32
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD11	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD12	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD13	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD11	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD12	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD13	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD11	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD12	6	0.25	0.09	0.24
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD13	6	0.25	0.09	0.24
(1,1647)	1:128:D:LEU:HD11	2:290:G:TRP:HE3	6	0.25	0.09	0.24
(1,1647)	1:128:D:LEU:HD12	2:290:G:TRP:HE3	6	0.25	0.09	0.24
(1,1647)	1:128:D:LEU:HD13	2:290:G:TRP:HE3	6	0.25	0.09	0.24
(1,1647)	1:128:D:LEU:HD21	2:290:G:TRP:HE3	6	0.25	0.09	0.24
(1,1647)	1:128:D:LEU:HD22	2:290:G:TRP:HE3	6	0.25	0.09	0.24
(1,1647)	1:128:D:LEU:HD23	2:290:G:TRP:HE3	6	0.25	0.09	0.24
(1,297)	1:95:A:ALA:H	1:98:A:LEU:H	6	0.24	0.18	0.17
(1,565)	1:60:B:LEU:H	1:82:B:GLY:H	6	0.24	0.09	0.22
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD11	6	0.22	0.09	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD12	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD13	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD21	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD22	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD23	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD11	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD12	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD13	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD21	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD22	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD23	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD11	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD12	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD13	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD21	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD22	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD23	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD11	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD12	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD13	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD21	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD22	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD23	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD11	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD12	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD13	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD21	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD22	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD23	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD11	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD12	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD13	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD21	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD22	6	0.22	0.09	0.2
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD23	6	0.22	0.09	0.2
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD21	6	0.22	0.12	0.19
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD22	6	0.22	0.12	0.19
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD23	6	0.22	0.12	0.19
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD21	6	0.22	0.12	0.19
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD22	6	0.22	0.12	0.19
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD23	6	0.22	0.12	0.19
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD21	6	0.22	0.12	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD22	6	0.22	0.12	0.19
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD23	6	0.22	0.12	0.19
(1,1042)	1:98:C:LEU:H	1:99:C:GLY:H	6	0.22	0.06	0.22
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE1	6	0.21	0.08	0.18
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE2	6	0.21	0.08	0.18
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE1	6	0.21	0.08	0.18
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE2	6	0.21	0.08	0.18
(1,1637)	1:98:D:LEU:HD11	2:281:G:PHE:HZ	6	0.2	0.05	0.19
(1,1637)	1:98:D:LEU:HD12	2:281:G:PHE:HZ	6	0.2	0.05	0.19
(1,1637)	1:98:D:LEU:HD13	2:281:G:PHE:HZ	6	0.2	0.05	0.19
(1,1637)	1:98:D:LEU:HD21	2:281:G:PHE:HZ	6	0.2	0.05	0.19
(1,1637)	1:98:D:LEU:HD22	2:281:G:PHE:HZ	6	0.2	0.05	0.19
(1,1637)	1:98:D:LEU:HD23	2:281:G:PHE:HZ	6	0.2	0.05	0.19
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD11	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD12	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD13	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD11	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD12	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD13	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD11	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD12	6	0.2	0.08	0.16
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD13	6	0.2	0.08	0.16
(1,498)	1:44:B:LEU:H	1:63:B:THR:H	6	0.2	0.06	0.22
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG21	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG22	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG23	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG21	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG22	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG23	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG21	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG22	6	0.18	0.06	0.2
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG23	6	0.18	0.06	0.2
(1,285)	1:92:A:THR:H	1:94:A:MET:H	6	0.18	0.13	0.13
(1,995)	1:77:C:GLU:H	1:78:C:VAL:H	6	0.17	0.03	0.16
(1,1155)	1:17:D:TYR:H	1:81:D:GLY:H	6	0.17	0.04	0.17
(1,682)	1:110:B:ALA:H	1:112:B:GLU:H	6	0.17	0.07	0.15
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG21	6	0.16	0.02	0.15
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG22	6	0.16	0.02	0.15
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG23	6	0.16	0.02	0.15
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG21	6	0.16	0.02	0.15
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG22	6	0.16	0.02	0.15
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG23	6	0.16	0.02	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG21	6	0.16	0.02	0.15
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG22	6	0.16	0.02	0.15
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG23	6	0.16	0.02	0.15
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD11	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD12	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD13	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD11	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD12	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD13	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD11	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD12	6	0.16	0.04	0.16
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD13	6	0.16	0.04	0.16
(1,1594)	1:128:C:LEU:HD11	2:290:F:TRP:HE3	6	0.15	0.05	0.13
(1,1594)	1:128:C:LEU:HD12	2:290:F:TRP:HE3	6	0.15	0.05	0.13
(1,1594)	1:128:C:LEU:HD13	2:290:F:TRP:HE3	6	0.15	0.05	0.13
(1,1594)	1:128:C:LEU:HD21	2:290:F:TRP:HE3	6	0.15	0.05	0.13
(1,1594)	1:128:C:LEU:HD22	2:290:F:TRP:HE3	6	0.15	0.05	0.13
(1,1594)	1:128:C:LEU:HD23	2:290:F:TRP:HE3	6	0.15	0.05	0.13
(1,909)	1:55:C:VAL:H	1:86:C:ILE:H	6	0.15	0.03	0.15
(1,116)	1:42:A:LEU:HD21	1:44:A:LEU:H	5	2.07	0.4	2.04
(1,116)	1:42:A:LEU:HD22	1:44:A:LEU:H	5	2.07	0.4	2.04
(1,116)	1:42:A:LEU:HD23	1:44:A:LEU:H	5	2.07	0.4	2.04
(1,87)	1:32:A:PHE:HD1	1:36:A:TRP:HZ3	5	1.49	1.28	1.15
(1,87)	1:32:A:PHE:HD2	1:36:A:TRP:HZ3	5	1.49	1.28	1.15
(1,872)	1:44:C:LEU:HD11	1:63:C:THR:H	5	0.87	0.33	0.92
(1,872)	1:44:C:LEU:HD12	1:63:C:THR:H	5	0.87	0.33	0.92
(1,872)	1:44:C:LEU:HD13	1:63:C:THR:H	5	0.87	0.33	0.92
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD11	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD12	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD13	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD11	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD12	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD13	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD11	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD12	5	0.68	0.58	0.39
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD13	5	0.68	0.58	0.39
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD21	5	0.63	0.42	0.37
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD22	5	0.63	0.42	0.37
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD23	5	0.63	0.42	0.37
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD21	5	0.63	0.42	0.37
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD22	5	0.63	0.42	0.37
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD23	5	0.63	0.42	0.37

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD21	5	0.63	0.42	0.37
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD22	5	0.63	0.42	0.37
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD23	5	0.63	0.42	0.37
(1,475)	1:36:B:TRP:HE3	1:37:B:GLN:H	5	0.62	0.49	0.38
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD21	5	0.5	0.58	0.23
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD22	5	0.5	0.58	0.23
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD23	5	0.5	0.58	0.23
(1,468)	1:34:B:LYS:H	1:35:B:ASP:H	5	0.47	0.28	0.66
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD21	5	0.46	0.21	0.44
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD22	5	0.46	0.21	0.44
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD23	5	0.46	0.21	0.44
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG21	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG22	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG23	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG21	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG22	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG23	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG21	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG22	5	0.4	0.26	0.24
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG23	5	0.4	0.26	0.24
(1,521)	1:51:B:LEU:H	1:57:B:GLU:H	5	0.34	0.15	0.3
(1,1022)	1:91:C:GLY:H	1:95:C:ALA:H	5	0.33	0.14	0.32
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD1	5	0.3	0.12	0.29
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD2	5	0.3	0.12	0.29
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD1	5	0.3	0.12	0.29
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD2	5	0.3	0.12	0.29
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD1	5	0.3	0.12	0.29
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD2	5	0.3	0.12	0.29
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG11	5	0.3	0.15	0.29
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG12	5	0.3	0.15	0.29
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG13	5	0.3	0.15	0.29
(1,496)	1:43:B:ASP:H	1:65:B:THR:H	5	0.27	0.06	0.3
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD1	5	0.26	0.07	0.29
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD2	5	0.26	0.07	0.29
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD1	5	0.26	0.07	0.29
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD2	5	0.26	0.07	0.29
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD1	5	0.26	0.07	0.29
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD2	5	0.26	0.07	0.29
(1,1382)	1:91:D:GLY:H	1:95:D:ALA:H	5	0.25	0.11	0.2
(1,357)	1:121:A:GLY:H	1:123:A:PHE:H	5	0.25	0.08	0.26
(1,111)	1:41:A:LYS:H	1:65:A:THR:H	5	0.25	0.1	0.2
(1,840)	1:36:C:TRP:H	1:37:C:GLN:H	5	0.23	0.04	0.23

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,303)	1:97:A:CYS:H	1:98:A:LEU:H	5	0.21	0.05	0.22
(1,1050)	1:99:C:GLY:H	1:102:C:CYS:H	5	0.21	0.11	0.16
(1,1462)	1:128:D:LEU:HD11	1:129:D:ALA:H	5	0.21	0.06	0.21
(1,1462)	1:128:D:LEU:HD12	1:129:D:ALA:H	5	0.21	0.06	0.21
(1,1462)	1:128:D:LEU:HD13	1:129:D:ALA:H	5	0.21	0.06	0.21
(1,506)	1:45:B:ASP:H	1:63:B:THR:H	5	0.21	0.08	0.19
(1,1412)	1:99:D:GLY:H	1:102:D:CYS:H	5	0.2	0.09	0.23
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD11	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD12	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD13	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD21	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD22	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD23	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD11	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD12	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD13	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD21	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD22	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD23	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD11	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD12	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD13	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD21	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD22	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD23	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD11	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD12	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD13	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD21	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD22	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD23	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD11	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD12	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD13	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD21	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD22	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD23	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD11	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD12	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD13	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD21	5	0.2	0.1	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD22	5	0.2	0.1	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD23	5	0.2	0.1	0.15
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD11	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD12	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD13	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD21	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD22	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD23	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD11	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD12	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD13	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD21	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD22	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD23	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD11	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD12	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD13	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD21	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD22	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD23	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD11	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD12	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD13	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD21	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD22	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD23	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD11	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD12	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD13	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD21	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD22	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD23	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD11	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD12	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD13	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD21	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD22	5	0.19	0.06	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD23	5	0.19	0.06	0.19
(1,1028)	1:93:C:GLN:H	1:96:C:HIS:H	5	0.19	0.07	0.18
(1,1541)	1:128:A:LEU:HD11	2:290:E:TRP:HE3	5	0.19	0.04	0.2
(1,1541)	1:128:A:LEU:HD12	2:290:E:TRP:HE3	5	0.19	0.04	0.2
(1,1541)	1:128:A:LEU:HD13	2:290:E:TRP:HE3	5	0.19	0.04	0.2
(1,1541)	1:128:A:LEU:HD21	2:290:E:TRP:HE3	5	0.19	0.04	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1541)	1:128:A:LEU:HD22	2:290:E:TRP:HE3	5	0.19	0.04	0.2
(1,1541)	1:128:A:LEU:HD23	2:290:E:TRP:HE3	5	0.19	0.04	0.2
(1,1469)	1:133:D:PHE:H	1:135:D:ALA:H	5	0.18	0.06	0.18
(1,146)	1:50:A:GLN:H	1:57:A:GLU:H	5	0.18	0.04	0.18
(1,50)	1:23:A:PHE:H	1:21:B:ILE:H	5	0.18	0.06	0.17
(1,376)	1:133:A:PHE:H	1:134:A:ASP:H	5	0.17	0.03	0.15
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG21	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG22	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG23	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG21	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG22	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG23	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG21	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG22	5	0.17	0.03	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG23	5	0.17	0.03	0.17
(1,961)	1:66:C:ALA:H	1:73:C:ALA:H	5	0.17	0.02	0.17
(1,319)	1:101:A:TYR:H	1:102:A:CYS:H	5	0.16	0.03	0.17
(1,413)	1:12:B:GLN:H	1:13:B:ILE:H	5	0.15	0.03	0.14
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD11	5	0.15	0.02	0.15
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD12	5	0.15	0.02	0.15
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD13	5	0.15	0.02	0.15
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD11	5	0.15	0.04	0.13
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD12	5	0.15	0.04	0.13
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD13	5	0.15	0.04	0.13
(2,2)	1:40:C:VAL:O	2:290:F:TRP:NE1	5	0.15	0.03	0.14
(1,1007)	1:82:C:GLY:H	1:83:C:ILE:H	5	0.14	0.02	0.14
(1,1659)	1:60:B:LEU:HD21	2:281:H:PHE:HZ	5	0.14	0.02	0.14
(1,1659)	1:60:B:LEU:HD22	2:281:H:PHE:HZ	5	0.14	0.02	0.14
(1,1659)	1:60:B:LEU:HD23	2:281:H:PHE:HZ	5	0.14	0.02	0.14
(1,553)	1:58:B:VAL:HG11	1:59:B:VAL:H	5	0.14	0.04	0.12
(1,553)	1:58:B:VAL:HG12	1:59:B:VAL:H	5	0.14	0.04	0.12
(1,553)	1:58:B:VAL:HG13	1:59:B:VAL:H	5	0.14	0.04	0.12
(1,913)	1:56:C:TYR:H	1:85:C:SER:H	5	0.14	0.01	0.13
(1,696)	1:115:B:THR:H	1:116:B:SER:H	5	0.12	0.02	0.12
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	5	0.12	0.02	0.11
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	5	0.12	0.02	0.11
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	5	0.12	0.02	0.11
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	5	0.12	0.02	0.11
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	5	0.12	0.02	0.11
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	5	0.12	0.02	0.11
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	5	0.12	0.02	0.11
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	5	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	5	0.12	0.02	0.11
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD21	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD22	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD23	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD21	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD22	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD23	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD21	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD22	4	1.58	0.72	1.23
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD23	4	1.58	0.72	1.23
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD11	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD12	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD13	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD11	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD12	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD13	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD11	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD12	4	1.38	1.13	0.88
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD13	4	1.38	1.13	0.88
(1,94)	1:36:A:TRP:HE3	1:37:A:GLN:H	4	1.21	0.47	1.04
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	4	1.13	0.79	0.98
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	4	1.13	0.79	0.98
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD21	4	1.04	0.77	0.89
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD22	4	1.04	0.77	0.89
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD23	4	1.04	0.77	0.89
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	4	0.86	0.35	0.9
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	4	0.86	0.35	0.9
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG11	4	0.79	0.24	0.77

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG12	4	0.79	0.24	0.77
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG13	4	0.79	0.24	0.77
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG11	4	0.79	0.24	0.77
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG12	4	0.79	0.24	0.77
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG13	4	0.79	0.24	0.77
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG11	4	0.79	0.24	0.77
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG12	4	0.79	0.24	0.77
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG13	4	0.79	0.24	0.77
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG21	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG22	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG23	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG21	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG22	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG23	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG21	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG22	4	0.78	0.29	0.64
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG23	4	0.78	0.29	0.64
(1,824)	1:31:C:VAL:HG11	1:32:C:PHE:H	4	0.65	0.14	0.66
(1,824)	1:31:C:VAL:HG12	1:32:C:PHE:H	4	0.65	0.14	0.66
(1,824)	1:31:C:VAL:HG13	1:32:C:PHE:H	4	0.65	0.14	0.66
(1,1046)	1:98:C:LEU:HD11	1:99:C:GLY:H	4	0.39	0.29	0.34
(1,1046)	1:98:C:LEU:HD12	1:99:C:GLY:H	4	0.39	0.29	0.34
(1,1046)	1:98:C:LEU:HD13	1:99:C:GLY:H	4	0.39	0.29	0.34
(1,1138)	1:10:D:THR:H	1:89:D:ILE:H	4	0.38	0.05	0.38
(1,716)	1:125:B:GLN:H	1:125:C:GLN:H	4	0.36	0.04	0.36
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB1	4	0.35	0.22	0.28
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB2	4	0.35	0.22	0.28
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB3	4	0.35	0.22	0.28
(1,550)	1:58:B:VAL:H	1:84:B:PHE:H	4	0.34	0.04	0.34
(1,641)	1:92:B:THR:H	1:95:B:ALA:H	4	0.32	0.18	0.3
(1,777)	1:17:C:TYR:HE1	1:82:C:GLY:H	4	0.29	0.1	0.3
(1,777)	1:17:C:TYR:HE2	1:82:C:GLY:H	4	0.29	0.1	0.3
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG11	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG12	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG13	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG11	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG12	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG13	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG11	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG12	4	0.28	0.21	0.18
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG13	4	0.28	0.21	0.18
(1,384)	1:135:A:ALA:H	1:138:A:MET:H	4	0.28	0.09	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,750)	1:139:B:ASN:H	1:141:B:LEU:H	4	0.26	0.11	0.22
(1,1019)	1:90:C:GLU:H	1:94:C:MET:H	4	0.23	0.09	0.24
(1,1176)	1:24:D:GLU:H	1:75:D:LEU:H	4	0.23	0.1	0.2
(1,370)	1:128:A:LEU:HD21	1:129:A:ALA:H	4	0.22	0.1	0.2
(1,370)	1:128:A:LEU:HD22	1:129:A:ALA:H	4	0.22	0.1	0.2
(1,370)	1:128:A:LEU:HD23	1:129:A:ALA:H	4	0.22	0.1	0.2
(1,441)	1:23:B:PHE:H	1:24:B:GLU:H	4	0.22	0.04	0.22
(1,644)	1:93:B:GLN:H	1:96:B:HIS:H	4	0.22	0.09	0.2
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG21	4	0.22	0.05	0.21
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG22	4	0.22	0.05	0.21
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG23	4	0.22	0.05	0.21
(1,3)	1:10:A:THR:H	1:87:A:ALA:H	4	0.22	0.11	0.18
(1,876)	1:45:C:ASP:H	1:63:C:THR:H	4	0.21	0.06	0.21
(1,748)	1:138:B:MET:H	1:141:B:LEU:H	4	0.21	0.09	0.16
(1,922)	1:58:C:VAL:H	1:84:C:PHE:H	4	0.21	0.01	0.22
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG21	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG22	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG23	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG21	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG22	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG23	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG21	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG22	4	0.21	0.03	0.2
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG23	4	0.21	0.03	0.2
(1,302)	1:96:A:HIS:H	1:99:A:GLY:H	4	0.19	0.07	0.16
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD11	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD12	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD13	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD21	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD22	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD23	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD11	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD12	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD13	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD21	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD22	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD23	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD11	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD12	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD13	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD21	4	0.19	0.06	0.18
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD22	4	0.19	0.06	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD23	4	0.19	0.06	0.18
(1,1666)	1:129:B:ALA:HB1	2:290:H:TRP:HZ3	4	0.19	0.07	0.18
(1,1666)	1:129:B:ALA:HB2	2:290:H:TRP:HZ3	4	0.19	0.07	0.18
(1,1666)	1:129:B:ALA:HB3	2:290:H:TRP:HZ3	4	0.19	0.07	0.18
(1,821)	1:30:C:HIS:H	1:32:C:PHE:H	4	0.18	0.02	0.18
(1,136)	1:47:A:ALA:H	1:59:A:VAL:H	4	0.18	0.05	0.18
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG21	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG22	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG23	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG21	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG22	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG23	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG21	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG22	4	0.18	0.07	0.15
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG23	4	0.18	0.07	0.15
(1,1033)	1:95:C:ALA:H	1:98:C:LEU:H	4	0.17	0.08	0.14
(1,396)	1:138:A:MET:H	1:141:A:LEU:H	4	0.17	0.03	0.18
(1,1047)	1:99:C:GLY:H	1:100:C:ALA:H	4	0.16	0.01	0.16
(1,84)	1:32:A:PHE:H	1:33:A:GLN:H	4	0.16	0.04	0.16
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD11	4	0.15	0.02	0.15
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD12	4	0.15	0.02	0.15
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD13	4	0.15	0.02	0.15
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD11	4	0.15	0.02	0.15
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD12	4	0.15	0.02	0.15
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD13	4	0.15	0.02	0.15
(1,1200)	1:32:D:PHE:H	1:34:D:LYS:H	4	0.14	0.03	0.15
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD11	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD12	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD13	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD21	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD22	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD23	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD11	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD12	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD13	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD21	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD22	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD23	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD11	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD12	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD13	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD21	4	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)
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD22	4	0.14	0.03	0.14
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD23	4	0.14	0.03	0.14
(1,290)	1:94:A:MET:H	1:95:A:ALA:H	4	0.14	0.02	0.12
(1,697)	1:115:B:THR:H	1:117:B:MET:H	4	0.14	0.03	0.12
(1,1338)	1:73:D:ALA:H	1:74:D:PHE:H	4	0.13	0.03	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD11	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD12	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD13	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD21	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD22	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD23	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD11	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD12	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD13	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD21	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD22	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD23	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD11	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD12	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD13	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD21	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD22	4	0.12	0.01	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD23	4	0.12	0.01	0.12
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE1	3	3.71	0.44	3.64
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE2	3	3.71	0.44	3.64
(1,826)	1:31:C:VAL:HG11	1:36:C:TRP:HZ3	3	2.34	1.42	2.61
(1,826)	1:31:C:VAL:HG12	1:36:C:TRP:HZ3	3	2.34	1.42	2.61
(1,826)	1:31:C:VAL:HG13	1:36:C:TRP:HZ3	3	2.34	1.42	2.61
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	3	1.51	0.76	1.4
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	3	1.51	0.76	1.4
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	3	1.51	0.76	1.4
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	3	1.51	0.76	1.4
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	3	1.51	0.76	1.4
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	3	1.51	0.76	1.4
(1,941)	1:60:C:LEU:HD11	1:61:C:ARG:H	3	1.13	0.09	1.18
(1,941)	1:60:C:LEU:HD12	1:61:C:ARG:H	3	1.13	0.09	1.18
(1,941)	1:60:C:LEU:HD13	1:61:C:ARG:H	3	1.13	0.09	1.18
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	3	0.68	0.23	0.67
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	3	0.68	0.23	0.67
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	3	0.68	0.23	0.67
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	3	0.68	0.23	0.67
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	3	0.68	0.23	0.67

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	3	0.68	0.23	0.67
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	3	0.68	0.23	0.67
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	3	0.68	0.23	0.67
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	3	0.68	0.23	0.67
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	3	0.67	0.49	0.32
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	3	0.67	0.49	0.32
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	3	0.67	0.49	0.32
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	3	0.67	0.49	0.32
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	3	0.67	0.49	0.32
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	3	0.67	0.49	0.32
(1,1292)	1:60:D:LEU:HD11	1:62:D:VAL:H	3	0.65	0.18	0.76
(1,1292)	1:60:D:LEU:HD12	1:62:D:VAL:H	3	0.65	0.18	0.76
(1,1292)	1:60:D:LEU:HD13	1:62:D:VAL:H	3	0.65	0.18	0.76
(1,1225)	1:42:D:LEU:HD21	1:43:D:ASP:H	3	0.64	0.1	0.64
(1,1225)	1:42:D:LEU:HD22	1:43:D:ASP:H	3	0.64	0.1	0.64
(1,1225)	1:42:D:LEU:HD23	1:43:D:ASP:H	3	0.64	0.1	0.64
(1,233)	1:68:A:LEU:HD11	1:73:A:ALA:H	3	0.59	0.08	0.64
(1,233)	1:68:A:LEU:HD12	1:73:A:ALA:H	3	0.59	0.08	0.64
(1,233)	1:68:A:LEU:HD13	1:73:A:ALA:H	3	0.59	0.08	0.64
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	3	0.55	0.3	0.73
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	3	0.55	0.3	0.73
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	3	0.55	0.3	0.73
(1,115)	1:42:A:LEU:HD21	1:43:A:ASP:H	3	0.49	0.29	0.52
(1,115)	1:42:A:LEU:HD22	1:43:A:ASP:H	3	0.49	0.29	0.52
(1,115)	1:42:A:LEU:HD23	1:43:A:ASP:H	3	0.49	0.29	0.52
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE1	3	0.4	0.25	0.29
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE2	3	0.4	0.25	0.29
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE1	3	0.4	0.25	0.29
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE2	3	0.4	0.25	0.29
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE1	3	0.4	0.25	0.29
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE2	3	0.4	0.25	0.29
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD1	3	0.39	0.13	0.41
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD2	3	0.39	0.13	0.41
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD1	3	0.39	0.13	0.41
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD2	3	0.39	0.13	0.41
(1,464)	1:32:B:PHE:H	1:34:B:LYS:H	3	0.36	0.12	0.28
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD11	3	0.34	0.14	0.43
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD12	3	0.34	0.14	0.43
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD13	3	0.34	0.14	0.43
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD11	3	0.34	0.14	0.43
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD12	3	0.34	0.14	0.43
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD13	3	0.34	0.14	0.43

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	3	0.32	0.17	0.29
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	3	0.32	0.17	0.29
(1,99)	1:39:A:GLU:H	1:67:A:SER:H	3	0.29	0.1	0.34
(1,1088)	1:118:C:VAL:HG21	1:126:C:LEU:H	3	0.27	0.02	0.27
(1,1088)	1:118:C:VAL:HG22	1:126:C:LEU:H	3	0.27	0.02	0.27
(1,1088)	1:118:C:VAL:HG23	1:126:C:LEU:H	3	0.27	0.02	0.27
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD21	3	0.26	0.09	0.32
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD22	3	0.26	0.09	0.32
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD23	3	0.26	0.09	0.32
(1,523)	1:51:B:LEU:HD21	1:57:B:GLU:H	3	0.26	0.01	0.26
(1,523)	1:51:B:LEU:HD22	1:57:B:GLU:H	3	0.26	0.01	0.26
(1,523)	1:51:B:LEU:HD23	1:57:B:GLU:H	3	0.26	0.01	0.26
(1,1014)	1:87:C:ALA:H	1:89:C:ILE:H	3	0.24	0.15	0.17
(1,131)	1:45:A:ASP:H	1:62:A:VAL:H	3	0.23	0.12	0.16
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE1	3	0.22	0.09	0.24
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE2	3	0.22	0.09	0.24
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE3	3	0.22	0.09	0.24
(1,381)	1:134:A:ASP:H	1:136:A:LEU:H	3	0.21	0.08	0.19
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE1	3	0.2	0.01	0.2
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE2	3	0.2	0.01	0.2
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE1	3	0.2	0.01	0.2
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE2	3	0.2	0.01	0.2
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE1	3	0.2	0.01	0.2
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE2	3	0.2	0.01	0.2
(1,594)	1:68:B:LEU:H	1:71:B:GLU:H	3	0.2	0.04	0.23
(1,284)	1:92:A:THR:H	1:93:A:GLN:H	3	0.2	0.04	0.18
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD1	3	0.2	0.05	0.18
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD2	3	0.2	0.05	0.18
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD1	3	0.2	0.05	0.18
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD2	3	0.2	0.05	0.18
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD1	3	0.2	0.05	0.18
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD2	3	0.2	0.05	0.18
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB1	3	0.19	0.07	0.2
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB2	3	0.19	0.07	0.2
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB3	3	0.19	0.07	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD11	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD12	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD13	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD21	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD22	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD23	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD11	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD12	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD13	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD21	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD22	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD23	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD11	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD12	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD13	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD21	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD22	3	0.19	0.02	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD23	3	0.19	0.02	0.18
(1,1136)	1:10:D:THR:H	1:87:D:ALA:H	3	0.19	0.07	0.17
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD11	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD12	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD13	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD21	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD22	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD23	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD11	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD12	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD13	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD21	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD22	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD23	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD11	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD12	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD13	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD21	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD22	3	0.19	0.04	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD23	3	0.19	0.04	0.18
(1,1118)	1:135:C:ALA:H	1:138:C:MET:H	3	0.19	0.05	0.22
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE1	3	0.18	0.05	0.15
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE2	3	0.18	0.05	0.15
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE1	3	0.18	0.05	0.15
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE2	3	0.18	0.05	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD11	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD12	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD13	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD21	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD22	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD23	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD11	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD12	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD13	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD21	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD22	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD23	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD11	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD12	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD13	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD21	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD22	3	0.18	0.03	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD23	3	0.18	0.03	0.19
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD11	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD12	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD13	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD21	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD22	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD23	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD11	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD12	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD13	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD21	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD22	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD23	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD11	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD12	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD13	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD21	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD22	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD23	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD11	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD12	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD13	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD21	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD22	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD23	3	0.18	0.02	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD11	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD12	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD13	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD21	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD22	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD23	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD11	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD12	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD13	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD21	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD22	3	0.18	0.02	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD23	3	0.18	0.02	0.17
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG21	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG22	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG23	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG21	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG22	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG23	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG21	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG22	3	0.18	0.04	0.18
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG23	3	0.18	0.04	0.18
(1,547)	1:57:B:GLU:H	1:84:B:PHE:H	3	0.17	0.03	0.16
(1,960)	1:66:C:ALA:H	1:67:C:SER:H	3	0.17	0.03	0.16
(1,1095)	1:122:C:THR:H	1:18:D:THR:H	3	0.16	0.05	0.13
(1,24)	1:17:A:TYR:H	1:81:A:GLY:H	3	0.16	0.05	0.15
(1,1433)	1:113:D:CYS:H	1:115:D:THR:H	3	0.16	0.04	0.14
(1,1700)	1:128:B:LEU:HD11	2:290:H:TRP:HE3	3	0.16	0.05	0.14
(1,1700)	1:128:B:LEU:HD12	2:290:H:TRP:HE3	3	0.16	0.05	0.14
(1,1700)	1:128:B:LEU:HD13	2:290:H:TRP:HE3	3	0.16	0.05	0.14
(1,1700)	1:128:B:LEU:HD21	2:290:H:TRP:HE3	3	0.16	0.05	0.14
(1,1700)	1:128:B:LEU:HD22	2:290:H:TRP:HE3	3	0.16	0.05	0.14
(1,1700)	1:128:B:LEU:HD23	2:290:H:TRP:HE3	3	0.16	0.05	0.14
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD11	3	0.15	0.03	0.14
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD12	3	0.15	0.03	0.14
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD13	3	0.15	0.03	0.14
(1,499)	1:44:B:LEU:HD11	1:45:B:ASP:H	3	0.15	0.06	0.12
(1,499)	1:44:B:LEU:HD12	1:45:B:ASP:H	3	0.15	0.06	0.12
(1,499)	1:44:B:LEU:HD13	1:45:B:ASP:H	3	0.15	0.06	0.12
(1,1147)	1:14:D:GLN:H	1:15:D:ARG:H	3	0.15	0.02	0.14
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB1	3	0.14	0.01	0.14
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB2	3	0.14	0.01	0.14
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB3	3	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)
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB1	3	0.14	0.01	0.14
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB2	3	0.14	0.01	0.14
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB3	3	0.14	0.01	0.14
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB1	3	0.14	0.01	0.14
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB2	3	0.14	0.01	0.14
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB3	3	0.14	0.01	0.14
(1,1482)	1:136:D:LEU:H	1:137:D:PHE:H	3	0.14	0.03	0.13
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE1	3	0.14	0.03	0.15
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE2	3	0.14	0.03	0.15
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE3	3	0.14	0.03	0.15
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE1	3	0.14	0.03	0.15
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE2	3	0.14	0.03	0.15
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE3	3	0.14	0.03	0.15
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD11	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD12	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD13	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD11	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD12	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD13	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD11	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD12	3	0.13	0.01	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD13	3	0.13	0.01	0.14
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD11	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD12	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD13	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD21	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD22	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD23	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD11	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD12	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD13	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD21	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD22	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD23	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD11	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD12	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD13	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD21	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD22	3	0.13	0.01	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD23	3	0.13	0.01	0.13
(1,1038)	1:97:C:CYS:H	1:98:C:LEU:H	3	0.13	0.0	0.13
(1,198)	1:62:A:VAL:H	1:63:A:THR:H	3	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,557)	1:59:B:VAL:H	1:60:B:LEU:H	3	0.12	0.0	0.12
(1,657)	1:97:B:CYS:H	1:98:B:LEU:H	3	0.12	0.01	0.11
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB1	3	0.12	0.01	0.12
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB2	3	0.12	0.01	0.12
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB3	3	0.12	0.01	0.12
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB1	3	0.12	0.01	0.12
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB2	3	0.12	0.01	0.12
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB3	3	0.12	0.01	0.12
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB1	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB2	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB3	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB1	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB2	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB3	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB1	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB2	3	0.12	0.02	0.11
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB3	3	0.12	0.02	0.11
(1,1304)	1:64:D:VAL:H	1:65:D:THR:H	3	0.12	0.02	0.11
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD21	3	0.12	0.01	0.12
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD22	3	0.12	0.01	0.12
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD23	3	0.12	0.01	0.12
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG21	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG22	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG23	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG21	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG22	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG23	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG21	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG22	3	0.12	0.01	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG23	3	0.12	0.01	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD11	3	0.11	0.0	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD12	3	0.11	0.0	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD13	3	0.11	0.0	0.11
(1,932)	1:59:C:VAL:H	1:60:C:LEU:H	3	0.11	0.01	0.11
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB1	3	0.11	0.01	0.11
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB2	3	0.11	0.01	0.11
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB3	3	0.11	0.01	0.11
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB1	3	0.11	0.01	0.11
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB2	3	0.11	0.01	0.11
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB3	3	0.11	0.01	0.11
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG21	2	1.59	0.02	1.59
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG22	2	1.59	0.02	1.59

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG23	2	1.59	0.02	1.59
(1,1291)	1:60:D:LEU:HD11	1:61:D:ARG:H	2	1.37	0.01	1.37
(1,1291)	1:60:D:LEU:HD12	1:61:D:ARG:H	2	1.37	0.01	1.37
(1,1291)	1:60:D:LEU:HD13	1:61:D:ARG:H	2	1.37	0.01	1.37
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG21	2	1.12	0.05	1.12
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG22	2	1.12	0.05	1.12
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG23	2	1.12	0.05	1.12
(1,194)	1:60:A:LEU:HD11	1:61:A:ARG:H	2	1.06	0.21	1.06
(1,194)	1:60:A:LEU:HD12	1:61:A:ARG:H	2	1.06	0.21	1.06
(1,194)	1:60:A:LEU:HD13	1:61:A:ARG:H	2	1.06	0.21	1.06
(1,78)	1:31:A:VAL:HG11	1:123:A:PHE:HE1	2	0.97	0.26	0.97
(1,78)	1:31:A:VAL:HG11	1:123:A:PHE:HE2	2	0.97	0.26	0.97
(1,78)	1:31:A:VAL:HG12	1:123:A:PHE:HE1	2	0.97	0.26	0.97
(1,78)	1:31:A:VAL:HG12	1:123:A:PHE:HE2	2	0.97	0.26	0.97
(1,78)	1:31:A:VAL:HG13	1:123:A:PHE:HE1	2	0.97	0.26	0.97
(1,78)	1:31:A:VAL:HG13	1:123:A:PHE:HE2	2	0.97	0.26	0.97
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD21	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD22	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD23	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD21	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD22	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD23	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD21	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD22	2	0.86	0.68	0.86
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD23	2	0.86	0.68	0.86
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB1	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB2	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB3	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB1	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB2	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB3	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB1	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB2	2	0.67	0.52	0.67
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB3	2	0.67	0.52	0.67
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB1	2	0.64	0.2	0.64
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB2	2	0.64	0.2	0.64
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB3	2	0.64	0.2	0.64
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB1	2	0.64	0.2	0.64
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB2	2	0.64	0.2	0.64
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB3	2	0.64	0.2	0.64
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB1	2	0.64	0.2	0.64
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB2	2	0.64	0.2	0.64

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB3	2	0.64	0.2	0.64
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD21	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD22	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD23	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD21	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD22	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD23	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD21	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD22	2	0.6	0.09	0.6
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD23	2	0.6	0.09	0.6
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD11	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD12	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD13	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD11	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD12	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD13	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD11	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD12	2	0.57	0.09	0.57
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD13	2	0.57	0.09	0.57
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG11	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG12	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG13	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG11	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG12	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG13	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG11	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG12	2	0.54	0.16	0.54
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG13	2	0.54	0.16	0.54
(1,830)	1:31:C:VAL:HG21	1:123:C:PHE:HE1	2	0.52	0.03	0.52
(1,830)	1:31:C:VAL:HG21	1:123:C:PHE:HE2	2	0.52	0.03	0.52
(1,830)	1:31:C:VAL:HG22	1:123:C:PHE:HE1	2	0.52	0.03	0.52
(1,830)	1:31:C:VAL:HG22	1:123:C:PHE:HE2	2	0.52	0.03	0.52
(1,830)	1:31:C:VAL:HG23	1:123:C:PHE:HE1	2	0.52	0.03	0.52
(1,830)	1:31:C:VAL:HG23	1:123:C:PHE:HE2	2	0.52	0.03	0.52
(1,1108)	1:131:C:VAL:HG11	1:133:C:PHE:H	2	0.5	0.06	0.5
(1,1108)	1:131:C:VAL:HG12	1:133:C:PHE:H	2	0.5	0.06	0.5
(1,1108)	1:131:C:VAL:HG13	1:133:C:PHE:H	2	0.5	0.06	0.5
(1,414)	1:12:B:GLN:H	1:85:B:SER:H	2	0.48	0.04	0.48
(1,825)	1:31:C:VAL:HG11	1:32:C:PHE:HD1	2	0.46	0.13	0.46
(1,825)	1:31:C:VAL:HG11	1:32:C:PHE:HD2	2	0.46	0.13	0.46
(1,825)	1:31:C:VAL:HG12	1:32:C:PHE:HD1	2	0.46	0.13	0.46
(1,825)	1:31:C:VAL:HG12	1:32:C:PHE:HD2	2	0.46	0.13	0.46

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,825)	1:31:C:VAL:HG13	1:32:C:PHE:HD1	2	0.46	0.13	0.46
(1,825)	1:31:C:VAL:HG13	1:32:C:PHE:HD2	2	0.46	0.13	0.46
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG11	2	0.42	0.01	0.42
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG12	2	0.42	0.01	0.42
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG13	2	0.42	0.01	0.42
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG11	2	0.42	0.01	0.42
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG12	2	0.42	0.01	0.42
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG13	2	0.42	0.01	0.42
(1,462)	1:31:B:VAL:HG21	1:123:B:PHE:HE1	2	0.38	0.26	0.38
(1,462)	1:31:B:VAL:HG21	1:123:B:PHE:HE2	2	0.38	0.26	0.38
(1,462)	1:31:B:VAL:HG22	1:123:B:PHE:HE1	2	0.38	0.26	0.38
(1,462)	1:31:B:VAL:HG22	1:123:B:PHE:HE2	2	0.38	0.26	0.38
(1,462)	1:31:B:VAL:HG23	1:123:B:PHE:HE1	2	0.38	0.26	0.38
(1,462)	1:31:B:VAL:HG23	1:123:B:PHE:HE2	2	0.38	0.26	0.38
(1,19)	1:14:A:GLN:H	1:85:A:SER:H	2	0.35	0.01	0.35
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD21	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD22	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD23	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD21	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD22	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD23	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD21	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD22	2	0.32	0.02	0.32
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD23	2	0.32	0.02	0.32
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD21	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD22	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD23	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD21	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD22	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD23	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD21	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD22	2	0.31	0.2	0.31
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD23	2	0.31	0.2	0.31
(1,171)	1:56:A:TYR:H	1:86:A:ILE:H	2	0.3	0.2	0.3
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG11	2	0.3	0.14	0.3
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG12	2	0.3	0.14	0.3
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG13	2	0.3	0.14	0.3
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD11	2	0.29	0.13	0.29
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD12	2	0.29	0.13	0.29
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD13	2	0.29	0.13	0.29
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD11	2	0.29	0.13	0.29
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD12	2	0.29	0.13	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD13	2	0.29	0.13	0.29
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD11	2	0.29	0.13	0.29
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD12	2	0.29	0.13	0.29
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD13	2	0.29	0.13	0.29
(1,446)	1:24:B:GLU:H	1:75:B:LEU:H	2	0.28	0.12	0.28
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD11	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD12	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD13	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD21	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD22	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD23	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD11	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD12	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD13	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD21	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD22	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD23	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD11	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD12	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD13	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD21	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD22	2	0.26	0.1	0.26
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD23	2	0.26	0.1	0.26
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG21	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG22	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG23	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG21	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG22	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG23	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG21	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG22	2	0.26	0.05	0.26
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG23	2	0.26	0.05	0.26
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD11	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD12	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD13	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD21	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD22	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD23	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD11	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD12	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD13	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD21	2	0.25	0.02	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD22	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD23	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD11	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD12	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD13	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD21	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD22	2	0.25	0.02	0.25
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD23	2	0.25	0.02	0.25
(1,1474)	1:134:D:ASP:H	1:137:D:PHE:H	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD21	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD22	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD23	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD21	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD22	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD23	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD21	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD22	2	0.24	0.08	0.24
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD23	2	0.24	0.08	0.24
(1,148)	1:51:A:LEU:H	1:55:A:VAL:H	2	0.24	0.08	0.24
(1,660)	1:97:B:CYS:H	1:101:B:TYR:H	2	0.24	0.06	0.24
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG21	2	0.24	0.03	0.24
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG22	2	0.24	0.03	0.24
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG23	2	0.24	0.03	0.24
(1,1248)	1:49:D:SER:H	1:59:D:VAL:H	2	0.23	0.12	0.23
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD11	2	0.22	0.11	0.22
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD12	2	0.22	0.11	0.22
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD13	2	0.22	0.11	0.22
(1,466)	1:33:B:GLN:H	1:34:B:LYS:H	2	0.22	0.03	0.22
(1,732)	1:134:B:ASP:H	1:136:B:LEU:H	2	0.22	0.12	0.22
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD11	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD12	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD13	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD21	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD22	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD23	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD11	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD12	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD13	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD21	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD22	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD23	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD11	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)
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD12	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD13	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD21	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD22	2	0.2	0.02	0.2
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD23	2	0.2	0.02	0.2
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD11	2	0.2	0.09	0.2
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD12	2	0.2	0.09	0.2
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD13	2	0.2	0.09	0.2
(1,1668)	1:40:B:VAL:HG11	2:290:H:TRP:HE1	2	0.2	0.04	0.2
(1,1668)	1:40:B:VAL:HG12	2:290:H:TRP:HE1	2	0.2	0.04	0.2
(1,1668)	1:40:B:VAL:HG13	2:290:H:TRP:HE1	2	0.2	0.04	0.2
(1,1186)	1:30:D:HIS:H	1:32:D:PHE:H	2	0.2	0.04	0.2
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE1	2	0.2	0.04	0.2
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE2	2	0.2	0.04	0.2
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE3	2	0.2	0.04	0.2
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE1	2	0.2	0.04	0.2
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE2	2	0.2	0.04	0.2
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE3	2	0.2	0.04	0.2
(2,1)	1:40:A:VAL:O	2:290:E:TRP:NE1	2	0.2	0.04	0.2
(1,670)	1:100:B:ALA:H	1:101:B:TYR:H	2	0.19	0.08	0.19
(1,658)	1:97:B:CYS:H	1:99:B:GLY:H	2	0.18	0.06	0.18
(1,1458)	1:126:D:LEU:H	1:127:D:ASN:H	2	0.18	0.06	0.18
(1,228)	1:67:A:SER:H	1:73:A:ALA:H	2	0.18	0.03	0.18
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG11	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG12	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG13	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG11	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG12	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG13	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG11	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG12	2	0.18	0.02	0.18
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG13	2	0.18	0.02	0.18
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD11	2	0.18	0.06	0.18
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD12	2	0.18	0.06	0.18
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD13	2	0.18	0.06	0.18
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD11	2	0.18	0.06	0.18
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD12	2	0.18	0.06	0.18
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD13	2	0.18	0.06	0.18
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD11	2	0.18	0.0	0.18
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD12	2	0.18	0.0	0.18
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD13	2	0.18	0.0	0.18
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD11	2	0.18	0.0	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD12	2	0.18	0.0	0.18
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD13	2	0.18	0.0	0.18
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD11	2	0.18	0.0	0.18
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD12	2	0.18	0.0	0.18
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD13	2	0.18	0.0	0.18
(1,546)	1:57:B:GLU:H	1:58:B:VAL:H	2	0.17	0.03	0.17
(1,738)	1:136:B:LEU:H	1:138:B:MET:H	2	0.17	0.03	0.17
(1,1122)	1:136:C:LEU:H	1:139:C:ASN:H	2	0.17	0.0	0.17
(1,1045)	1:98:C:LEU:H	1:102:C:CYS:H	2	0.17	0.07	0.17
(1,1409)	1:99:D:GLY:H	1:100:D:ALA:H	2	0.17	0.04	0.17
(1,1507)	1:129:A:ALA:HB1	2:290:E:TRP:HZ3	2	0.17	0.01	0.17
(1,1507)	1:129:A:ALA:HB2	2:290:E:TRP:HZ3	2	0.17	0.01	0.17
(1,1507)	1:129:A:ALA:HB3	2:290:E:TRP:HZ3	2	0.17	0.01	0.17
(1,322)	1:109:A:TYR:H	1:111:A:ARG:H	2	0.16	0.06	0.16
(1,325)	1:110:A:ALA:H	1:112:A:GLU:H	2	0.16	0.03	0.16
(1,1442)	1:116:D:SER:H	1:118:D:VAL:H	2	0.16	0.01	0.16
(1,421)	1:15:B:ARG:H	1:83:B:ILE:H	2	0.16	0.05	0.16
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD11	2	0.16	0.02	0.16
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD12	2	0.16	0.02	0.16
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD13	2	0.16	0.02	0.16
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD11	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD12	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD13	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD21	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD22	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD23	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD11	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD12	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD13	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD21	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD22	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD23	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD11	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD12	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD13	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD21	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD22	2	0.15	0.01	0.15
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD23	2	0.15	0.01	0.15
(1,455)	1:31:B:VAL:H	1:32:B:PHE:H	2	0.15	0.04	0.15
(1,1562)	1:40:C:VAL:HG11	2:290:F:TRP:HE1	2	0.15	0.0	0.15
(1,1562)	1:40:C:VAL:HG12	2:290:F:TRP:HE1	2	0.15	0.0	0.15
(1,1562)	1:40:C:VAL:HG13	2:290:F:TRP:HE1	2	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1405)	1:97:D:CYS:H	1:100:D:ALA:H	2	0.15	0.0	0.15
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG21	2	0.14	0.02	0.14
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG22	2	0.14	0.02	0.14
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG23	2	0.14	0.02	0.14
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG21	2	0.14	0.02	0.14
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG22	2	0.14	0.02	0.14
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG23	2	0.14	0.02	0.14
(1,765)	1:14:C:GLN:H	1:15:C:ARG:H	2	0.14	0.02	0.14
(1,698)	1:116:B:SER:H	1:117:B:MET:H	2	0.13	0.02	0.13
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG21	2	0.13	0.01	0.13
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG22	2	0.13	0.01	0.13
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG23	2	0.13	0.01	0.13
(1,217)	1:66:A:ALA:H	1:67:A:SER:H	2	0.12	0.01	0.12
(1,305)	1:97:A:CYS:H	1:100:A:ALA:H	2	0.12	0.01	0.12
(1,1610)	1:106:D:LEU:HD11	2:281:G:PHE:HZ	2	0.12	0.02	0.12
(1,1610)	1:106:D:LEU:HD12	2:281:G:PHE:HZ	2	0.12	0.02	0.12
(1,1610)	1:106:D:LEU:HD13	2:281:G:PHE:HZ	2	0.12	0.02	0.12
(1,801)	1:23:C:PHE:H	1:24:C:GLU:H	2	0.12	0.01	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD11	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD12	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD13	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD11	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD12	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD13	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD11	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD12	2	0.12	0.0	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD13	2	0.12	0.0	0.12
(1,1614)	1:126:D:LEU:HD11	2:290:G:TRP:HZ2	2	0.12	0.0	0.12
(1,1614)	1:126:D:LEU:HD12	2:290:G:TRP:HZ2	2	0.12	0.0	0.12
(1,1614)	1:126:D:LEU:HD13	2:290:G:TRP:HZ2	2	0.12	0.0	0.12
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE1	2	0.12	0.0	0.12
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE2	2	0.12	0.0	0.12
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE3	2	0.12	0.0	0.12
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE1	2	0.12	0.0	0.12
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE2	2	0.12	0.0	0.12
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE3	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD11	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD12	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD13	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD21	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD22	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD23	2	0.12	0.0	0.12

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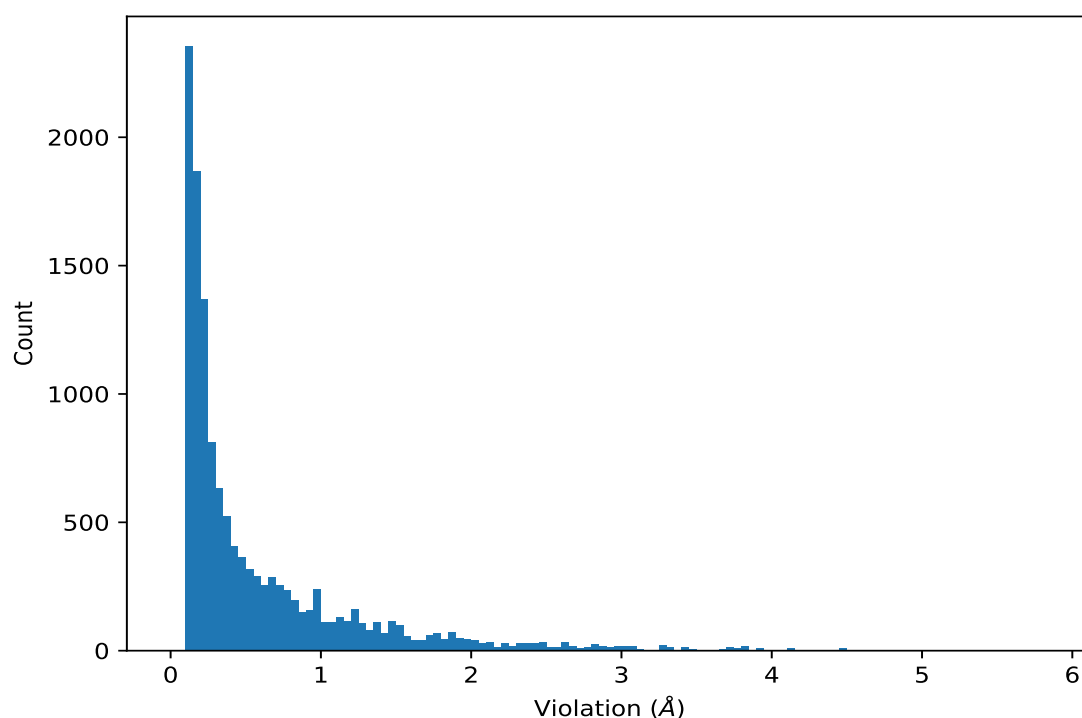
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD11	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD12	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD13	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD21	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD22	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD23	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD11	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD12	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD13	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD21	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD22	2	0.12	0.0	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD23	2	0.12	0.0	0.12
(1,646)	1:94:B:MET:H	1:96:B:HIS:H	2	0.11	0.01	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG11	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG12	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG13	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG11	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG12	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG13	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG11	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG12	2	0.11	0.0	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG13	2	0.11	0.0	0.11
(1,1185)	1:30:D:HIS:H	1:31:D:VAL:H	2	0.11	0.0	0.11
(1,163)	1:54:A:ASP:H	1:55:A:VAL:H	2	0.1	0.0	0.1

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	6	5.82
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	6	5.82
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	6	5.82
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	13	5.68
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	13	5.68
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	13	5.68
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	18	5.38
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	18	5.38
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	18	5.38
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	6	4.69
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	6	4.69
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	6	4.69
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	15	4.48
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	15	4.48
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	15	4.48
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	15	4.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	15	4.48
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	15	4.48
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	15	4.48
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	15	4.48
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	15	4.48
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE1	2	4.27
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE2	2	4.27
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	4	4.13
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	4	4.13
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	4	4.13
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	4	4.13
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	4	4.13
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	4	4.13
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	4	4.13
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	4	4.13
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	4	4.13
(1,826)	1:31:C:VAL:HG11	1:36:C:TRP:HZ3	6	3.92
(1,826)	1:31:C:VAL:HG12	1:36:C:TRP:HZ3	6	3.92
(1,826)	1:31:C:VAL:HG13	1:36:C:TRP:HZ3	6	3.92
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	15	3.9
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	15	3.9
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	15	3.9
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	15	3.9
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	15	3.9
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	15	3.9
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	2	3.83
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	2	3.83
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	2	3.83
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	2	3.83
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	2	3.83
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	2	3.83
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	2	3.83
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	2	3.83
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	2	3.83
(1,87)	1:32:A:PHE:HD1	1:36:A:TRP:HZ3	6	3.83
(1,87)	1:32:A:PHE:HD2	1:36:A:TRP:HZ3	6	3.83
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	17	3.8
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	17	3.8
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	17	3.8
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	17	3.8
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	17	3.8
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	17	3.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	14	3.75
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	14	3.75
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	14	3.75
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	14	3.75
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	14	3.75
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	14	3.75
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	14	3.75
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	14	3.75
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	14	3.75
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	19	3.73
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	19	3.73
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	19	3.73
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	19	3.73
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	19	3.73
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	19	3.73
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	1	3.73
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	1	3.73
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	1	3.73
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	1	3.73
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	1	3.73
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	1	3.73
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	1	3.73
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	1	3.73
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	1	3.73
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	13	3.66
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	13	3.66
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	13	3.66
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	18	3.66
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	18	3.66
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	18	3.66
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE1	13	3.64
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE2	13	3.64
(1,371)	1:131:A:VAL:H	1:133:A:PHE:HE1	17	3.53
(1,371)	1:131:A:VAL:H	1:133:A:PHE:HE2	17	3.53
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	6	3.49
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	3	3.48
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	3	3.48
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	3	3.48
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	3	3.48
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	3	3.48
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	3	3.48
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	6	3.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	6	3.42
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	6	3.42
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	6	3.42
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	6	3.42
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	6	3.42
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	12	3.4
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	12	3.4
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	12	3.4
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	12	3.4
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	12	3.4
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	12	3.4
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	16	3.32
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	16	3.32
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	16	3.32
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	16	3.32
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	16	3.32
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	16	3.32
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	15	3.3
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	15	3.3
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	15	3.3
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	15	3.3
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	15	3.3
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	15	3.3
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	15	3.3
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	15	3.3
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	15	3.3
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	16	3.29
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	16	3.29
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	16	3.29
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	16	3.29
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	16	3.29
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	16	3.29
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	16	3.29
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	16	3.29
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	16	3.29
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE1	2	3.29
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE2	2	3.29
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD11	9	3.27
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD12	9	3.27
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD13	9	3.27
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD11	9	3.27
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD12	9	3.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD13	9	3.27
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD11	9	3.27
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD12	9	3.27
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD13	9	3.27
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE1	7	3.21
(1,164)	1:54:A:ASP:H	1:56:A:TYR:HE2	7	3.21
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	7	3.14
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	7	3.14
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	7	3.14
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	7	3.14
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	7	3.14
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	7	3.14
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	10	3.06
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	10	3.06
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	10	3.06
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	10	3.06
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	10	3.06
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	10	3.06
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	10	3.06
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	10	3.06
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	10	3.06
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	9	3.05
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	9	3.05
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	9	3.05
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	9	3.05
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	9	3.05
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	9	3.05
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	9	3.05
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	9	3.05
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	9	3.05
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	20	3.02
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	20	3.02
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	20	3.02
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	20	3.02
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	20	3.02
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	20	3.02
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	20	3.02
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	20	3.02
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	20	3.02
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	19	3.01
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	19	3.01
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	19	3.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	19	3.01
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	19	3.01
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	19	3.01
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	19	3.01
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	19	3.01
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	19	3.01
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	7	3.0
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE1	2	2.97
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE2	2	2.97
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE3	2	2.97
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE1	2	2.97
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE2	2	2.97
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE3	2	2.97
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	14	2.97
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	14	2.97
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	14	2.97
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	14	2.97
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	14	2.97
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	14	2.97
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	15	2.96
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	15	2.96
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	15	2.96
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE1	13	2.95
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE2	13	2.95
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	2	2.94
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	2	2.94
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	2	2.94
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	7	2.92
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	7	2.92
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	7	2.92
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	7	2.92
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	7	2.92
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	7	2.92
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	7	2.92
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	7	2.92
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	7	2.92
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	14	2.9
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	14	2.9
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	14	2.9
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	10	2.89
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	10	2.89
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	10	2.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	16	2.86
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	16	2.86
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	16	2.86
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	13	2.86
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	13	2.86
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	13	2.86
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	13	2.86
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	13	2.86
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	13	2.86
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	13	2.86
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	13	2.86
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	13	2.86
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	15	2.85
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	15	2.85
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	15	2.85
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD21	15	2.82
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD22	15	2.82
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD23	15	2.82
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD21	15	2.82
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD22	15	2.82
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD23	15	2.82
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD21	15	2.82
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD22	15	2.82
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD23	15	2.82
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	12	2.82
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	12	2.82
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	12	2.82
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	12	2.82
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	12	2.82
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	12	2.82
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	12	2.82
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	12	2.82
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	12	2.82
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	12	2.8
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	12	2.8
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	12	2.8
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	14	2.8
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	14	2.8
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	14	2.8
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	2	2.79
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	2	2.79
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	2	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	12	2.78
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	12	2.78
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	12	2.78
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	15	2.76
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	15	2.76
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	15	2.76
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	15	2.76
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	6	2.75
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	6	2.75
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	6	2.75
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	16	2.74
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	16	2.74
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	16	2.74
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE1	7	2.74
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE2	7	2.74
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	3	2.71
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	3	2.71
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	3	2.71
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	16	2.7
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	16	2.7
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	16	2.7
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	9	2.69
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	9	2.69
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	9	2.69
(1,116)	1:42:A:LEU:HD21	1:44:A:LEU:H	13	2.69
(1,116)	1:42:A:LEU:HD22	1:44:A:LEU:H	13	2.69
(1,116)	1:42:A:LEU:HD23	1:44:A:LEU:H	13	2.69
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	15	2.65
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	15	2.65
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	15	2.65
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	12	2.65
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	12	2.65
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	12	2.65
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	12	2.65
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	12	2.65
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	12	2.65
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	12	2.65
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	12	2.65
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	12	2.65
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	15	2.63
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	15	2.63
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	15	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	15	2.63
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	15	2.63
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	15	2.63
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE1	20	2.62
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE2	20	2.62
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE3	20	2.62
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE1	20	2.62
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE2	20	2.62
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE3	20	2.62
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	18	2.62
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	18	2.62
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	18	2.62
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	18	2.62
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	18	2.62
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	18	2.62
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	18	2.62
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	18	2.62
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	18	2.62
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	17	2.61
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	17	2.61
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	17	2.61
(1,826)	1:31:C:VAL:HG11	1:36:C:TRP:HZ3	13	2.61
(1,826)	1:31:C:VAL:HG12	1:36:C:TRP:HZ3	13	2.61
(1,826)	1:31:C:VAL:HG13	1:36:C:TRP:HZ3	13	2.61
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	2	2.6
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	2	2.6
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	2	2.6
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	2	2.6
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	2	2.6
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	2	2.6
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	12	2.58
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	12	2.58
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	12	2.58
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	6	2.55
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	6	2.55
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	6	2.55
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	6	2.55
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	6	2.55
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	6	2.55
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	6	2.55
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	6	2.55
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	6	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	18	2.53
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	18	2.53
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	18	2.53
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	4	2.52
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	17	2.52
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	17	2.52
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	17	2.52
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	17	2.52
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	17	2.52
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	17	2.52
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	19	2.51
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	19	2.51
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	19	2.51
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	3	2.49
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	3	2.49
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	3	2.49
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	3	2.49
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	3	2.49
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	3	2.49
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	18	2.48
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	18	2.48
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	18	2.48
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	18	2.48
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	18	2.48
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	18	2.48
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	18	2.48
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	18	2.48
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	18	2.48
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	18	2.48
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	18	2.48
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	18	2.48
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	6	2.47
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	6	2.47
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	6	2.47
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	6	2.47
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	6	2.47
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	6	2.47
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	6	2.47
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	6	2.47
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	6	2.47
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	13	2.46
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	13	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	13	2.46
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	19	2.45
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	19	2.45
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	19	2.45
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	19	2.44
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	19	2.44
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	19	2.44
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	19	2.43
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	19	2.43
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	19	2.43
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	19	2.43
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	19	2.43
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	19	2.43
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	8	2.43
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	8	2.43
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	8	2.43
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	8	2.43
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	8	2.43
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	8	2.43
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	8	2.43
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	8	2.43
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	8	2.43
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	5	2.42
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	5	2.42
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	5	2.42
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	16	2.4
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	16	2.4
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	16	2.4
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	16	2.4
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	16	2.4
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	16	2.4
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	16	2.4
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	16	2.4
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	16	2.4
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	19	2.39
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	19	2.39
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	19	2.39
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	19	2.39
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	19	2.39
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	19	2.39
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	19	2.39
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	19	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	19	2.39
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	15	2.38
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	15	2.38
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	15	2.38
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	17	2.38
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	17	2.38
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	17	2.38
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	14	2.38
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	14	2.38
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	14	2.38
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	14	2.38
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	14	2.38
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	14	2.38
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	14	2.38
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	14	2.38
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	14	2.38
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	9	2.37
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	9	2.37
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	9	2.37
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	17	2.36
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	17	2.36
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	17	2.36
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	17	2.35
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	2	2.34
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	13	2.33
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	14	2.33
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	14	2.33
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	14	2.33
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	19	2.32
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	19	2.32
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	19	2.32
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	16	2.32
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	16	2.32
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	16	2.32
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	6	2.31
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	14	2.31
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	14	2.31
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	14	2.31
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	14	2.31
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	14	2.31
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	14	2.31
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	14	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	14	2.31
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	14	2.31
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	2	2.31
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	2	2.31
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	2	2.31
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	13	2.3
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	13	2.3
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	13	2.3
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	5	2.3
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	5	2.3
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	5	2.3
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	18	2.29
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	18	2.29
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	18	2.29
(1,116)	1:42:A:LEU:HD21	1:44:A:LEU:H	18	2.29
(1,116)	1:42:A:LEU:HD22	1:44:A:LEU:H	18	2.29
(1,116)	1:42:A:LEU:HD23	1:44:A:LEU:H	18	2.29
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	12	2.28
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	18	2.26
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	18	2.26
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	18	2.26
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	18	2.26
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	18	2.26
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	18	2.26
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	18	2.26
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	18	2.26
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	18	2.26
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	18	2.25
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	1	2.24
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	1	2.24
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	1	2.24
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	7	2.24
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	7	2.24
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	7	2.24
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	15	2.22
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	3	2.22
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	3	2.22
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	3	2.22
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	3	2.22
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	3	2.22
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	3	2.22
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	10	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	10	2.2
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	10	2.2
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	14	2.2
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	14	2.2
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	14	2.2
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	12	2.2
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	12	2.2
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	12	2.2
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	12	2.2
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	12	2.2
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	12	2.2
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	6	2.2
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	6	2.2
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	6	2.2
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD21	16	2.2
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD22	16	2.2
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD23	16	2.2
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	15	2.19
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	15	2.19
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	15	2.19
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	8	2.18
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	8	2.18
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	8	2.18
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	13	2.18
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	13	2.18
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	13	2.18
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	14	2.18
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	14	2.18
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	14	2.18
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	3	2.18
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	3	2.18
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	3	2.18
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	8	2.14
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	8	2.14
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	8	2.14
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD11	16	2.13
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD12	16	2.13
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD13	16	2.13
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	12	2.12
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	17	2.11
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	17	2.11
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	17	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	17	2.11
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	17	2.11
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	17	2.11
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	17	2.11
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	17	2.11
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	17	2.11
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	7	2.1
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	7	2.1
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	7	2.1
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	7	2.1
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	7	2.1
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	7	2.1
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	7	2.1
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	7	2.1
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	7	2.1
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	16	2.1
(1,566)	1:60:B:LEU:HD11	1:61:B:ARG:H	15	2.1
(1,566)	1:60:B:LEU:HD12	1:61:B:ARG:H	15	2.1
(1,566)	1:60:B:LEU:HD13	1:61:B:ARG:H	15	2.1
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	4	2.1
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	4	2.1
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	4	2.1
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	15	2.06
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	15	2.06
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	15	2.06
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	15	2.06
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	15	2.06
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	15	2.06
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	15	2.06
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	15	2.06
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	15	2.06
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	2	2.05
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	2	2.05
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	2	2.05
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	2	2.05
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	2	2.05
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	2	2.05
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	2	2.05
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	2	2.05
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	2	2.05
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	1	2.05
(1,566)	1:60:B:LEU:HD11	1:61:B:ARG:H	18	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:60:B:LEU:HD12	1:61:B:ARG:H	18	2.05
(1,566)	1:60:B:LEU:HD13	1:61:B:ARG:H	18	2.05
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	15	2.05
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	15	2.05
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	15	2.05
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	15	2.05
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	15	2.05
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	15	2.05
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	13	2.04
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	20	2.04
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	20	2.04
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	20	2.04
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	20	2.04
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	20	2.04
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	20	2.04
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	20	2.04
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	20	2.04
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	20	2.04
(1,116)	1:42:A:LEU:HD21	1:44:A:LEU:H	3	2.04
(1,116)	1:42:A:LEU:HD22	1:44:A:LEU:H	3	2.04
(1,116)	1:42:A:LEU:HD23	1:44:A:LEU:H	3	2.04
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	6	2.03
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	6	2.03
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	6	2.03
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	15	2.02
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	15	2.02
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	15	2.02
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	6	2.02
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	6	2.02
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	6	2.02
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	6	2.02
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	6	2.02
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	6	2.02
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	7	2.02
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	7	2.02
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	7	2.02
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	7	2.02
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	7	2.02
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	7	2.02
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	19	2.01
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD11	18	2.01
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD12	18	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD13	18	2.01
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	1	2.0
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	1	2.0
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	1	2.0
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	15	2.0
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	15	2.0
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	15	2.0
(1,94)	1:36:A:TRP:HE3	1:37:A:GLN:H	6	2.0
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	4	1.99
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	4	1.99
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	4	1.99
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	4	1.99
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	4	1.99
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	4	1.99
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	4	1.99
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	4	1.99
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	4	1.99
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	1	1.99
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	1	1.99
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	1	1.99
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	1	1.99
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	1	1.99
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	1	1.99
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	16	1.99
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	16	1.99
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	16	1.99
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	16	1.99
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	16	1.99
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	16	1.99
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	5	1.98
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	5	1.98
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	5	1.98
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	17	1.98
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	17	1.98
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	17	1.98
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	4	1.96
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	4	1.96
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	4	1.96
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	12	1.96
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	12	1.96
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	12	1.96
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	2	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	2	1.96
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	2	1.96
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	8	1.96
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	8	1.96
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	8	1.96
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	15	1.95
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	15	1.95
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	15	1.95
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	19	1.95
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	19	1.95
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	19	1.95
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	18	1.93
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	8	1.93
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	8	1.93
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	8	1.93
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	8	1.93
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	8	1.93
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	8	1.93
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	8	1.93
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	8	1.93
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	8	1.93
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	3	1.93
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	3	1.93
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	3	1.93
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	3	1.93
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	3	1.93
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	3	1.93
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	3	1.93
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	3	1.93
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	3	1.93
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	19	1.92
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	19	1.92
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	19	1.92
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	3	1.92
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	3	1.92
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	3	1.92
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	3	1.92
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	20	1.92
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	20	1.92
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	20	1.92
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	16	1.91
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	16	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	16	1.91
(1,870)	1:44:C:LEU:HD11	1:62:C:VAL:HG11	18	1.91
(1,870)	1:44:C:LEU:HD11	1:62:C:VAL:HG12	18	1.91
(1,870)	1:44:C:LEU:HD11	1:62:C:VAL:HG13	18	1.91
(1,870)	1:44:C:LEU:HD12	1:62:C:VAL:HG11	18	1.91
(1,870)	1:44:C:LEU:HD12	1:62:C:VAL:HG12	18	1.91
(1,870)	1:44:C:LEU:HD12	1:62:C:VAL:HG13	18	1.91
(1,870)	1:44:C:LEU:HD13	1:62:C:VAL:HG11	18	1.91
(1,870)	1:44:C:LEU:HD13	1:62:C:VAL:HG12	18	1.91
(1,870)	1:44:C:LEU:HD13	1:62:C:VAL:HG13	18	1.91
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	6	1.9
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	6	1.9
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	6	1.9
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	6	1.9
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	6	1.9
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	6	1.9
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	6	1.9
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	6	1.9
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	6	1.9
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	9	1.89
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	9	1.89
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	9	1.89
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	15	1.89
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	15	1.89
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	15	1.89
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	15	1.89
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	15	1.89
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	15	1.89
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	15	1.89
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	15	1.89
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	15	1.89
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	5	1.89
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	5	1.89
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	5	1.89
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	5	1.89
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	5	1.89
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	5	1.89
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	5	1.89
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	5	1.89
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	5	1.89
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	15	1.88
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	15	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	15	1.88
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	15	1.88
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	15	1.88
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	15	1.88
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	15	1.88
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	15	1.88
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	15	1.88
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	13	1.88
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	17	1.88
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	17	1.88
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	17	1.88
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	17	1.88
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	17	1.88
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	17	1.88
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	17	1.88
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	17	1.88
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	17	1.88
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	19	1.88
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	19	1.88
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	19	1.88
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	19	1.88
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	19	1.88
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	19	1.88
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	19	1.88
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	19	1.88
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	19	1.88
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD11	19	1.88
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD12	19	1.88
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD13	19	1.88
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD11	19	1.88
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD12	19	1.88
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD13	19	1.88
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD11	19	1.88
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD12	19	1.88
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD13	19	1.88
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	6	1.88
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	6	1.88
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	6	1.88
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	19	1.85
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	19	1.85
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	19	1.85
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	19	1.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	19	1.85
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	19	1.85
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	19	1.85
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	19	1.85
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	19	1.85
(1,566)	1:60:B:LEU:HD11	1:61:B:ARG:H	16	1.85
(1,566)	1:60:B:LEU:HD12	1:61:B:ARG:H	16	1.85
(1,566)	1:60:B:LEU:HD13	1:61:B:ARG:H	16	1.85
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	3	1.84
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	6	1.83
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	15	1.83
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	15	1.83
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	15	1.83
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	14	1.83
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	14	1.83
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	14	1.83
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	14	1.83
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	14	1.83
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	14	1.83
(1,566)	1:60:B:LEU:HD11	1:61:B:ARG:H	6	1.83
(1,566)	1:60:B:LEU:HD12	1:61:B:ARG:H	6	1.83
(1,566)	1:60:B:LEU:HD13	1:61:B:ARG:H	6	1.83
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	17	1.83
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	17	1.83
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	17	1.83
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	17	1.83
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	17	1.83
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	17	1.83
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	6	1.82
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	9	1.82
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	9	1.82
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	9	1.82
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	16	1.82
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	16	1.82
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	16	1.82
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	16	1.81
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	16	1.81
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	16	1.81
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	12	1.81
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	12	1.81
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	12	1.81
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE1	4	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE2	4	1.81
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE3	4	1.81
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE1	4	1.81
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE2	4	1.81
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE3	4	1.81
(1,566)	1:60:B:LEU:HD11	1:61:B:ARG:H	20	1.81
(1,566)	1:60:B:LEU:HD12	1:61:B:ARG:H	20	1.81
(1,566)	1:60:B:LEU:HD13	1:61:B:ARG:H	20	1.81
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	19	1.81
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	19	1.81
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	19	1.81
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	10	1.79
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	8	1.79
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	8	1.79
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	8	1.79
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	14	1.79
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	14	1.79
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	14	1.79
(1,116)	1:42:A:LEU:HD21	1:44:A:LEU:H	7	1.79
(1,116)	1:42:A:LEU:HD22	1:44:A:LEU:H	7	1.79
(1,116)	1:42:A:LEU:HD23	1:44:A:LEU:H	7	1.79
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	18	1.79
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	18	1.79
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	18	1.79
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	18	1.79
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	18	1.79
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	18	1.79
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	18	1.79
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	18	1.79
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	18	1.79
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	16	1.78
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	16	1.78
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	16	1.78
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	12	1.78
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	12	1.78
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	12	1.78
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	6	1.78
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	6	1.78
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	6	1.78
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	20	1.78
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	20	1.78
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	20	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	20	1.78
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	20	1.78
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	20	1.78
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	20	1.78
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	20	1.78
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	20	1.78
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	5	1.77
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	5	1.77
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	5	1.77
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	15	1.77
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	15	1.77
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	15	1.77
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	13	1.77
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	13	1.77
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	13	1.77
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	19	1.76
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	19	1.76
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	19	1.76
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	19	1.76
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	19	1.76
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	19	1.76
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	19	1.76
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	19	1.76
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	19	1.76
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	15	1.76
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	15	1.76
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	15	1.76
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	15	1.76
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	15	1.76
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	15	1.76
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	15	1.76
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	15	1.76
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	15	1.76
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	3	1.76
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	3	1.76
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	3	1.76
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	12	1.75
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	12	1.75
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	12	1.75
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	15	1.74
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	4	1.74
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	4	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	4	1.74
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD11	3	1.74
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD12	3	1.74
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD13	3	1.74
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD11	3	1.74
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD12	3	1.74
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD13	3	1.74
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD11	3	1.74
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD12	3	1.74
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD13	3	1.74
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	6	1.74
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	6	1.74
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	6	1.74
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	3	1.73
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	3	1.73
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	3	1.73
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	15	1.73
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	15	1.73
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	15	1.73
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	13	1.73
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	13	1.73
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	13	1.73
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD11	15	1.73
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD12	15	1.73
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD13	15	1.73
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD11	15	1.73
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD12	15	1.73
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD13	15	1.73
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD11	15	1.73
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD12	15	1.73
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD13	15	1.73
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	18	1.72
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	18	1.72
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	18	1.72
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	15	1.72
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	15	1.72
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	15	1.72
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	7	1.71
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	7	1.71
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	7	1.71
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	7	1.71
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	7	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	7	1.71
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	7	1.71
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	7	1.71
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	7	1.71
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	12	1.7
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	12	1.7
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	12	1.7
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	6	1.7
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	6	1.7
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	6	1.7
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	3	1.7
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	3	1.7
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	3	1.7
(1,566)	1:60:B:LEU:HD11	1:61:B:ARG:H	17	1.7
(1,566)	1:60:B:LEU:HD12	1:61:B:ARG:H	17	1.7
(1,566)	1:60:B:LEU:HD13	1:61:B:ARG:H	17	1.7
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	16	1.69
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	18	1.69
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	18	1.69
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	18	1.69
(1,87)	1:32:A:PHE:HD1	1:36:A:TRP:HZ3	10	1.69
(1,87)	1:32:A:PHE:HD2	1:36:A:TRP:HZ3	10	1.69
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	9	1.68
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	9	1.68
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	9	1.68
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	6	1.67
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	6	1.67
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	6	1.67
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	6	1.67
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	6	1.67
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	6	1.67
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	6	1.67
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	6	1.67
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	6	1.67
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	5	1.67
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	13	1.67
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	13	1.67
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	13	1.67
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	4	1.66
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	4	1.66
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	4	1.66
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	3	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	3	1.66
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	3	1.66
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	3	1.66
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	3	1.66
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	3	1.66
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	3	1.66
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	3	1.66
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	3	1.66
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	19	1.65
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	19	1.65
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	19	1.65
(1,535)	1:54:B:ASP:H	1:56:B:TYR:HE1	8	1.65
(1,535)	1:54:B:ASP:H	1:56:B:TYR:HE2	8	1.65
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD21	16	1.65
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD22	16	1.65
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD23	16	1.65
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	17	1.64
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	17	1.64
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	17	1.64
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	20	1.63
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	20	1.63
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	20	1.63
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	9	1.63
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	9	1.63
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	9	1.63
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	3	1.63
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	3	1.63
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	3	1.63
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	13	1.62
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	13	1.62
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	13	1.62
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	4	1.62
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	4	1.62
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	4	1.62
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	10	1.62
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	10	1.62
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	10	1.62
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD11	15	1.62
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD12	15	1.62
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD13	15	1.62
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	2	1.61
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	2	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	2	1.61
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG21	6	1.61
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG22	6	1.61
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG23	6	1.61
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	10	1.61
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	10	1.61
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	10	1.61
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	12	1.61
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	12	1.61
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	12	1.61
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	17	1.6
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	17	1.6
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	17	1.6
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	12	1.6
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	12	1.6
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	12	1.6
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	20	1.59
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	20	1.59
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	20	1.59
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	20	1.59
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	20	1.59
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	20	1.59
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	1	1.59
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	1	1.59
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	1	1.59
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	2	1.59
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	2	1.59
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	2	1.59
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	2	1.59
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	2	1.59
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	2	1.59
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	2	1.59
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	2	1.59
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	2	1.59
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	16	1.58
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	16	1.58
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	16	1.58
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	19	1.58
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	19	1.58
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	19	1.58
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	10	1.57
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	10	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	10	1.57
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG21	20	1.57
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG22	20	1.57
(1,1078)	1:116:C:SER:H	1:118:C:VAL:HG23	20	1.57
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	16	1.57
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	16	1.57
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	16	1.57
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	20	1.57
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	20	1.57
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	20	1.57
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	1	1.56
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	14	1.56
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	6	1.56
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	6	1.56
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	20	1.56
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	20	1.56
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	20	1.56
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	8	1.56
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	8	1.56
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	8	1.56
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	8	1.56
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	8	1.56
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	8	1.56
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	8	1.56
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	8	1.56
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	8	1.56
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	19	1.55
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	19	1.55
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	19	1.55
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	7	1.55
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	7	1.55
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	7	1.55
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD21	2	1.54
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD22	2	1.54
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD23	2	1.54
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD21	2	1.54
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD22	2	1.54
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD23	2	1.54
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD21	2	1.54
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD22	2	1.54
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD23	2	1.54
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	3	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	3	1.53
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	3	1.53
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	3	1.53
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	3	1.53
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	3	1.53
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	3	1.53
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	3	1.53
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	3	1.53
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	4	1.53
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	4	1.53
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	4	1.53
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	4	1.53
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	4	1.53
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	4	1.53
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	4	1.53
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	4	1.53
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	4	1.53
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	16	1.53
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	16	1.53
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	16	1.53
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	12	1.53
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	12	1.53
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	12	1.53
(1,467)	1:33:B:GLN:H	1:35:B:ASP:H	16	1.53
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	1	1.53
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	1	1.53
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	1	1.53
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	1	1.53
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	1	1.53
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	1	1.53
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	1	1.53
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	1	1.53
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	1	1.53
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	2	1.52
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	2	1.52
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	2	1.52
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	1	1.52
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	1	1.52
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	1	1.52
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	2	1.52
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	2	1.52
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	2	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	2	1.52
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	2	1.52
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	2	1.52
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	2	1.52
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	2	1.52
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	2	1.52
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	9	1.52
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	9	1.52
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	9	1.52
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	9	1.52
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	9	1.52
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	9	1.52
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	9	1.52
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	9	1.52
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	9	1.52
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	7	1.52
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	7	1.52
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	7	1.52
(1,368)	1:128:A:LEU:HD11	1:129:A:ALA:H	12	1.52
(1,368)	1:128:A:LEU:HD12	1:129:A:ALA:H	12	1.52
(1,368)	1:128:A:LEU:HD13	1:129:A:ALA:H	12	1.52
(1,116)	1:42:A:LEU:HD21	1:44:A:LEU:H	1	1.52
(1,116)	1:42:A:LEU:HD22	1:44:A:LEU:H	1	1.52
(1,116)	1:42:A:LEU:HD23	1:44:A:LEU:H	1	1.52
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	4	1.51
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD11	8	1.51
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD12	8	1.51
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD13	8	1.51
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD11	8	1.51
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD12	8	1.51
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD13	8	1.51
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD11	8	1.51
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD12	8	1.51
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD13	8	1.51
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	16	1.5
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	16	1.5
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	16	1.5
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	16	1.5
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	16	1.5
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	16	1.5
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	16	1.5
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	16	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	16	1.5
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	20	1.5
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	20	1.5
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	20	1.5
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	19	1.5
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	19	1.5
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	19	1.5
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	17	1.49
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	17	1.49
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	17	1.49
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	4	1.49
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	4	1.49
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	4	1.49
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	6	1.49
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	6	1.49
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	6	1.49
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	6	1.49
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	6	1.49
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	6	1.49
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	6	1.49
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	6	1.49
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	6	1.49
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	20	1.48
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	20	1.48
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	20	1.48
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	20	1.48
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	20	1.48
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	20	1.48
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	20	1.48
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	20	1.48
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	20	1.48
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	14	1.48
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	14	1.48
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	7	1.48
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	7	1.48
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	7	1.48
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	3	1.48
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	3	1.48
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	3	1.48
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	3	1.48
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	3	1.48
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	3	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	3	1.48
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	3	1.48
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	3	1.48
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	3	1.48
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	3	1.48
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	3	1.48
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	3	1.48
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	3	1.48
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	3	1.48
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	3	1.48
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	3	1.48
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	3	1.48
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	6	1.47
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	6	1.47
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	6	1.47
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	15	1.47
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	15	1.47
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	15	1.47
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	15	1.47
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	15	1.47
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	15	1.47
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	15	1.47
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	15	1.47
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	15	1.47
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	17	1.46
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	17	1.46
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	17	1.46
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	2	1.46
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	16	1.46
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	16	1.46
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	16	1.46
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	16	1.46
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	16	1.46
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	16	1.46
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	16	1.46
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	16	1.46
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	16	1.46
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	16	1.46
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	16	1.46
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	16	1.46
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	2	1.46
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	2	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	2	1.46
(1,538)	1:55:B:VAL:H	1:56:B:TYR:HE1	8	1.46
(1,538)	1:55:B:VAL:H	1:56:B:TYR:HE2	8	1.46
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD11	20	1.46
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD12	20	1.46
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD13	20	1.46
(1,467)	1:33:B:GLN:H	1:35:B:ASP:H	19	1.46
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	2	1.46
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	2	1.46
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	2	1.46
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	2	1.46
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	2	1.46
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	2	1.46
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	2	1.46
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	2	1.46
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	2	1.46
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	19	1.45
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	12	1.45
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	17	1.45
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	17	1.45
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	17	1.45
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	7	1.45
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	7	1.45
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	7	1.45
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	7	1.45
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	7	1.45
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	7	1.45
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	7	1.45
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	7	1.45
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	7	1.45
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD11	6	1.45
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD12	6	1.45
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD13	6	1.45
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	4	1.45
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	4	1.45
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	4	1.45
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	19	1.45
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	19	1.45
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	19	1.45
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	10	1.44
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	2	1.44
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	2	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	2	1.44
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	6	1.44
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	6	1.44
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	6	1.44
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	6	1.44
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	6	1.44
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	6	1.44
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	6	1.44
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	6	1.44
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	6	1.44
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	10	1.44
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	10	1.44
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	10	1.44
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	10	1.44
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	10	1.44
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	10	1.44
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	10	1.44
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	10	1.44
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	10	1.44
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	8	1.43
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	14	1.43
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	14	1.43
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	14	1.43
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	13	1.42
(1,872)	1:44:C:LEU:HD11	1:63:C:THR:H	18	1.42
(1,872)	1:44:C:LEU:HD12	1:63:C:THR:H	18	1.42
(1,872)	1:44:C:LEU:HD13	1:63:C:THR:H	18	1.42
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	20	1.41
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	20	1.41
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	20	1.41
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	16	1.41
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	16	1.41
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	16	1.41
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	16	1.41
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	16	1.41
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	16	1.41
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	16	1.41
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	16	1.41
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	16	1.41
(1,114)	1:42:A:LEU:HD11	1:128:A:LEU:HD21	1	1.41
(1,114)	1:42:A:LEU:HD11	1:128:A:LEU:HD22	1	1.41
(1,114)	1:42:A:LEU:HD11	1:128:A:LEU:HD23	1	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:42:A:LEU:HD12	1:128:A:LEU:HD21	1	1.41
(1,114)	1:42:A:LEU:HD12	1:128:A:LEU:HD22	1	1.41
(1,114)	1:42:A:LEU:HD12	1:128:A:LEU:HD23	1	1.41
(1,114)	1:42:A:LEU:HD13	1:128:A:LEU:HD21	1	1.41
(1,114)	1:42:A:LEU:HD13	1:128:A:LEU:HD22	1	1.41
(1,114)	1:42:A:LEU:HD13	1:128:A:LEU:HD23	1	1.41
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	7	1.4
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	7	1.4
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	7	1.4
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	12	1.4
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	8	1.4
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	8	1.4
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	8	1.4
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	8	1.4
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	8	1.4
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	8	1.4
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	4	1.4
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	4	1.4
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	4	1.4
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	4	1.4
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	4	1.4
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	4	1.4
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	4	1.4
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	4	1.4
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	4	1.4
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	9	1.39
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	9	1.39
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	9	1.39
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	9	1.39
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	9	1.39
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	9	1.39
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	9	1.39
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	9	1.39
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	9	1.39
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	12	1.39
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	18	1.39
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD21	20	1.39
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD22	20	1.39
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD23	20	1.39
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD21	20	1.39
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD22	20	1.39
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD23	20	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD21	20	1.39
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD22	20	1.39
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD23	20	1.39
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	7	1.39
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	7	1.39
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	7	1.39
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	5	1.39
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	5	1.39
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	5	1.39
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	6	1.38
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	6	1.38
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	6	1.38
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	14	1.38
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	14	1.38
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	14	1.38
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	4	1.38
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	4	1.38
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	4	1.38
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	7	1.38
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	7	1.38
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	7	1.38
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	18	1.38
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	2	1.38
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	2	1.38
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	2	1.38
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	8	1.38
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	8	1.38
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	8	1.38
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	8	1.38
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	8	1.38
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	8	1.38
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	8	1.38
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	8	1.38
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	8	1.38
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	12	1.37
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	12	1.37
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	12	1.37
(1,1291)	1:60:D:LEU:HD11	1:61:D:ARG:H	15	1.37
(1,1291)	1:60:D:LEU:HD12	1:61:D:ARG:H	15	1.37
(1,1291)	1:60:D:LEU:HD13	1:61:D:ARG:H	15	1.37
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	17	1.37
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	17	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	17	1.37
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	17	1.37
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	17	1.37
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	17	1.37
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	17	1.37
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	17	1.37
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	17	1.37
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	17	1.37
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	2	1.37
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	2	1.37
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	2	1.37
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	2	1.37
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	2	1.37
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	2	1.37
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	18	1.36
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	18	1.36
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	18	1.36
(1,1291)	1:60:D:LEU:HD11	1:61:D:ARG:H	13	1.36
(1,1291)	1:60:D:LEU:HD12	1:61:D:ARG:H	13	1.36
(1,1291)	1:60:D:LEU:HD13	1:61:D:ARG:H	13	1.36
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	18	1.36
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	18	1.36
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	18	1.36
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	16	1.36
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	3	1.36
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	3	1.36
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	3	1.36
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	3	1.36
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	3	1.36
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	3	1.36
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	16	1.36
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	16	1.36
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	16	1.36
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	15	1.36
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	15	1.36
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	15	1.36
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	14	1.36
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	16	1.36
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	16	1.36
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	16	1.36
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	4	1.35
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	4	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	4	1.35
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	4	1.35
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	4	1.35
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	4	1.35
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	4	1.35
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	4	1.35
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	4	1.35
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	9	1.35
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	4	1.35
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	18	1.35
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	7	1.34
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	6	1.34
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	6	1.34
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	6	1.34
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	6	1.34
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	6	1.34
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	6	1.34
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	9	1.34
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	9	1.34
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	9	1.34
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	9	1.34
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	9	1.34
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	9	1.34
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	14	1.34
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	14	1.34
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	14	1.34
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	9	1.34
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	9	1.34
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	9	1.34
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	7	1.33
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	7	1.33
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	7	1.33
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	7	1.33
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	7	1.33
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	7	1.33
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	7	1.33
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	7	1.33
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	7	1.33
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD21	5	1.33
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD22	5	1.33
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD23	5	1.33
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD21	5	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD22	5	1.33
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD23	5	1.33
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD21	5	1.33
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD22	5	1.33
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD23	5	1.33
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	17	1.32
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	17	1.32
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	17	1.32
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	17	1.32
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	17	1.32
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	17	1.32
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	17	1.32
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	17	1.32
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	17	1.32
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	3	1.32
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	3	1.32
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	3	1.32
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	16	1.32
(1,1130)	1:140:C:TYR:HD1	1:141:C:LEU:H	6	1.32
(1,1130)	1:140:C:TYR:HD2	1:141:C:LEU:H	6	1.32
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD11	10	1.32
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD12	10	1.32
(1,866)	1:43:C:ASP:H	1:44:C:LEU:HD13	10	1.32
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	4	1.32
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	4	1.32
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	4	1.32
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	1	1.31
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	1	1.31
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	1	1.31
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	3	1.31
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	3	1.31
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	3	1.31
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	5	1.31
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	5	1.31
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	5	1.31
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	1	1.31
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	1	1.31
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	1	1.31
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	1	1.31
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	1	1.31
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	1	1.31
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	1	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	1	1.31
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	1	1.31
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	20	1.3
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	20	1.3
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	20	1.3
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	20	1.29
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	20	1.29
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	20	1.29
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	20	1.29
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	20	1.29
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	20	1.29
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	20	1.29
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	20	1.29
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	20	1.29
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	8	1.29
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	11	1.29
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	10	1.28
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	10	1.28
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	10	1.28
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	2	1.28
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG21	9	1.28
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG22	9	1.28
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG23	9	1.28
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG21	9	1.28
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG22	9	1.28
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG23	9	1.28
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG21	9	1.28
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG22	9	1.28
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG23	9	1.28
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	3	1.28
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	3	1.28
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	3	1.28
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	16	1.27
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	16	1.27
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	16	1.27
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	16	1.27
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	16	1.27
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	16	1.27
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	16	1.27
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	16	1.27
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	16	1.27
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	1	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	1	1.27
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	1	1.27
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	1	1.27
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	1	1.27
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	1	1.27
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	1	1.27
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	1	1.27
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	1	1.27
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	3	1.27
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	3	1.27
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	3	1.27
(1,475)	1:36:B:TRP:HE3	1:37:B:GLN:H	10	1.27
(1,194)	1:60:A:LEU:HD11	1:61:A:ARG:H	14	1.27
(1,194)	1:60:A:LEU:HD12	1:61:A:ARG:H	14	1.27
(1,194)	1:60:A:LEU:HD13	1:61:A:ARG:H	14	1.27
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	20	1.26
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	10	1.26
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	4	1.26
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	4	1.26
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	4	1.26
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	4	1.26
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	4	1.26
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	4	1.26
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	6	1.26
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	6	1.26
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	6	1.26
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	9	1.26
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	9	1.26
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	9	1.26
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	18	1.26
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	18	1.26
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	18	1.26
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	1	1.26
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	1	1.26
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	1	1.26
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	3	1.26
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	3	1.26
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	3	1.26
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	1	1.26
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	1	1.26
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	1	1.26
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	1	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	1	1.26
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	1	1.26
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	1	1.26
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	1	1.26
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	1	1.26
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	17	1.25
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	17	1.25
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	17	1.25
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	17	1.25
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	17	1.25
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	17	1.25
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	17	1.25
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	17	1.25
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	17	1.25
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	19	1.25
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	1	1.25
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	1	1.25
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	1	1.25
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	8	1.25
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	8	1.25
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	8	1.25
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	18	1.25
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	18	1.25
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	18	1.25
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	8	1.25
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	8	1.25
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	8	1.25
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	8	1.25
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	8	1.25
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	8	1.25
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	4	1.24
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	4	1.24
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	4	1.24
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	3	1.24
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	6	1.24
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	6	1.24
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	6	1.24
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	2	1.24
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	2	1.24
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	2	1.24
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	14	1.24
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	14	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	14	1.24
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	12	1.24
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	12	1.24
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	12	1.24
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	12	1.24
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	12	1.24
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	12	1.24
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	12	1.24
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	12	1.24
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	12	1.24
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	15	1.24
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	15	1.24
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	15	1.24
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	19	1.24
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	5	1.24
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	20	1.23
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	20	1.23
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	20	1.23
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	20	1.23
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	20	1.23
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	20	1.23
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	20	1.23
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	20	1.23
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	20	1.23
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	18	1.23
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	20	1.23
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	20	1.23
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	20	1.23
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	20	1.23
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	20	1.23
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	20	1.23
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	20	1.23
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	20	1.23
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	20	1.23
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	7	1.23
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	7	1.23
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	7	1.23
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	7	1.23
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	7	1.23
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	7	1.23
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	7	1.23
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	7	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	7	1.23
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD21	17	1.23
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD22	17	1.23
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD23	17	1.23
(1,78)	1:31:A:VAL:HG11	1:123:A:PHE:HE1	20	1.23
(1,78)	1:31:A:VAL:HG11	1:123:A:PHE:HE2	20	1.23
(1,78)	1:31:A:VAL:HG12	1:123:A:PHE:HE1	20	1.23
(1,78)	1:31:A:VAL:HG12	1:123:A:PHE:HE2	20	1.23
(1,78)	1:31:A:VAL:HG13	1:123:A:PHE:HE1	20	1.23
(1,78)	1:31:A:VAL:HG13	1:123:A:PHE:HE2	20	1.23
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	5	1.22
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD11	6	1.22
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD12	6	1.22
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD13	6	1.22
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD11	6	1.22
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD12	6	1.22
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD13	6	1.22
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD11	6	1.22
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD12	6	1.22
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD13	6	1.22
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	16	1.22
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	16	1.22
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	16	1.22
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	16	1.22
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	16	1.22
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	16	1.22
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	16	1.22
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	16	1.22
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	16	1.22
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	1	1.22
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	1	1.22
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	1	1.22
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	11	1.22
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	11	1.22
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	11	1.22
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	10	1.22
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	10	1.22
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	10	1.22
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	7	1.21
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	7	1.21
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	7	1.21
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	5	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	5	1.21
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	5	1.21
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	5	1.21
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	5	1.21
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	5	1.21
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	5	1.21
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	5	1.21
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	5	1.21
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	8	1.21
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	8	1.21
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	8	1.21
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	8	1.21
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	8	1.21
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	8	1.21
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	8	1.21
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	8	1.21
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	8	1.21
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	18	1.21
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	3	1.21
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	12	1.21
(1,941)	1:60:C:LEU:HD11	1:61:C:ARG:H	13	1.21
(1,941)	1:60:C:LEU:HD12	1:61:C:ARG:H	13	1.21
(1,941)	1:60:C:LEU:HD13	1:61:C:ARG:H	13	1.21
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	14	1.21
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	14	1.21
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	14	1.21
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	14	1.21
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	14	1.21
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	14	1.21
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	14	1.21
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	14	1.21
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	14	1.21
(1,467)	1:33:B:GLN:H	1:35:B:ASP:H	17	1.21
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	4	1.21
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	4	1.21
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	4	1.21
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	4	1.21
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	4	1.21
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	4	1.21
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	4	1.21
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	4	1.21
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	4	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	2	1.2
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	2	1.2
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	2	1.2
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	2	1.2
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	2	1.2
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	2	1.2
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	2	1.2
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	2	1.2
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	2	1.2
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	13	1.2
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	13	1.2
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	13	1.2
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	3	1.2
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	3	1.2
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	3	1.2
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	3	1.2
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	3	1.2
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	3	1.2
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	3	1.2
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	3	1.2
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	3	1.2
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	6	1.2
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	4	1.19
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	4	1.19
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	4	1.19
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB1	16	1.19
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB2	16	1.19
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB3	16	1.19
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB1	16	1.19
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB2	16	1.19
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB3	16	1.19
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB1	16	1.19
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB2	16	1.19
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB3	16	1.19
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD1	13	1.19
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD2	13	1.19
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	4	1.18
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	5	1.18
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	5	1.18
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	5	1.18
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	5	1.18
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	5	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	5	1.18
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	5	1.18
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	5	1.18
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	5	1.18
(1,941)	1:60:C:LEU:HD11	1:61:C:ARG:H	4	1.18
(1,941)	1:60:C:LEU:HD12	1:61:C:ARG:H	4	1.18
(1,941)	1:60:C:LEU:HD13	1:61:C:ARG:H	4	1.18
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG21	6	1.17
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG22	6	1.17
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG23	6	1.17
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	12	1.17
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	12	1.17
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	12	1.17
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	12	1.17
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	12	1.17
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	12	1.17
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	12	1.17
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	12	1.17
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	12	1.17
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	13	1.17
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	10	1.17
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	10	1.17
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	10	1.17
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	1	1.17
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	1	1.17
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	1	1.17
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	12	1.17
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	12	1.17
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	12	1.17
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	8	1.16
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	8	1.16
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	8	1.16
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	8	1.16
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	8	1.16
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	8	1.16
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	8	1.16
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	8	1.16
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	8	1.16
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	10	1.16
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	10	1.16
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	10	1.16
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	10	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	10	1.16
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	10	1.16
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	10	1.16
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	10	1.16
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	10	1.16
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	18	1.16
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	18	1.16
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	18	1.16
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	8	1.16
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	8	1.16
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	8	1.16
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	8	1.16
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	8	1.16
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	8	1.16
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	8	1.16
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	8	1.16
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	8	1.16
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	9	1.16
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	9	1.16
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	9	1.16
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	9	1.16
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	9	1.16
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	9	1.16
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	10	1.16
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	10	1.16
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	10	1.16
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	10	1.16
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	10	1.16
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	10	1.16
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	6	1.15
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	2	1.15
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	2	1.15
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	2	1.15
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	17	1.15
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	17	1.15
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	17	1.15
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	9	1.15
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	9	1.15
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	9	1.15
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	9	1.15
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	9	1.15
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	9	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	9	1.15
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	9	1.15
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	9	1.15
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD11	17	1.15
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD12	17	1.15
(1,503)	1:45:B:ASP:H	1:60:B:LEU:HD13	17	1.15
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	14	1.15
(1,475)	1:36:B:TRP:HE3	1:37:B:GLN:H	9	1.15
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	7	1.15
(1,87)	1:32:A:PHE:HD1	1:36:A:TRP:HZ3	2	1.15
(1,87)	1:32:A:PHE:HD2	1:36:A:TRP:HZ3	2	1.15
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	1	1.14
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	1	1.14
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	1	1.14
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	1	1.14
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	1	1.14
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	1	1.14
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	1	1.14
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	1	1.14
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	1	1.14
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	4	1.14
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	4	1.14
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	4	1.14
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	4	1.14
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	4	1.14
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	4	1.14
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	4	1.14
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	4	1.14
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	4	1.14
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD21	17	1.14
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD22	17	1.14
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD23	17	1.14
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD21	17	1.14
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD22	17	1.14
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD23	17	1.14
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD21	17	1.14
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD22	17	1.14
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD23	17	1.14
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	10	1.14
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	10	1.14
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	10	1.14
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	14	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG11	6	1.13
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG12	6	1.13
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG13	6	1.13
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG11	6	1.13
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG12	6	1.13
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG13	6	1.13
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG11	6	1.13
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG12	6	1.13
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG13	6	1.13
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	7	1.13
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	16	1.13
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	16	1.13
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	16	1.13
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	19	1.13
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	19	1.13
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	19	1.13
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	20	1.13
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	20	1.13
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	20	1.13
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	14	1.13
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	14	1.13
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	14	1.13
(1,181)	1:58:A:VAL:HG11	1:60:A:LEU:HD21	9	1.13
(1,181)	1:58:A:VAL:HG11	1:60:A:LEU:HD22	9	1.13
(1,181)	1:58:A:VAL:HG11	1:60:A:LEU:HD23	9	1.13
(1,181)	1:58:A:VAL:HG12	1:60:A:LEU:HD21	9	1.13
(1,181)	1:58:A:VAL:HG12	1:60:A:LEU:HD22	9	1.13
(1,181)	1:58:A:VAL:HG12	1:60:A:LEU:HD23	9	1.13
(1,181)	1:58:A:VAL:HG13	1:60:A:LEU:HD21	9	1.13
(1,181)	1:58:A:VAL:HG13	1:60:A:LEU:HD22	9	1.13
(1,181)	1:58:A:VAL:HG13	1:60:A:LEU:HD23	9	1.13
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	7	1.13
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	7	1.13
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	7	1.13
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	7	1.13
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	7	1.13
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	7	1.13
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	7	1.13
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	7	1.13
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	7	1.13
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	7	1.12
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	7	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	7	1.12
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	14	1.12
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	14	1.12
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	14	1.12
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	18	1.12
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	18	1.12
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	18	1.12
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	20	1.12
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	16	1.12
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	9	1.12
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	12	1.12
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	9	1.11
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	12	1.11
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	12	1.11
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	12	1.11
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	19	1.11
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	19	1.11
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	19	1.11
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	19	1.11
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	19	1.11
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	19	1.11
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	20	1.11
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	20	1.11
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	20	1.11
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	20	1.11
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	20	1.11
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	20	1.11
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	20	1.11
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	20	1.11
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	20	1.11
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	16	1.11
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	16	1.11
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	16	1.11
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	16	1.11
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	16	1.11
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	16	1.11
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	16	1.11
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	16	1.11
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	16	1.11
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	5	1.11
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	5	1.11
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	5	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	5	1.11
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	5	1.11
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	5	1.11
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	5	1.11
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	5	1.11
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	5	1.11
(1,94)	1:36:A:TRP:HE3	1:37:A:GLN:H	2	1.11
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	2	1.1
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	2	1.1
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	2	1.1
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	2	1.1
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	2	1.1
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	2	1.1
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	2	1.1
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	2	1.1
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	2	1.1
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	6	1.1
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	12	1.09
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	12	1.09
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	12	1.09
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	12	1.09
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	12	1.09
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	12	1.09
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	18	1.09
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	18	1.09
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	18	1.09
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	18	1.09
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	18	1.09
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	18	1.09
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	18	1.09
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	18	1.09
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	18	1.09
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	20	1.09
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	20	1.09
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	20	1.09
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	4	1.09
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	4	1.09
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	4	1.09
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	13	1.09
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD1	2	1.09
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD2	2	1.09
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	12	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	12	1.08
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	12	1.08
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	12	1.08
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	12	1.08
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	12	1.08
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	12	1.08
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	12	1.08
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	12	1.08
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	7	1.08
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	17	1.08
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	16	1.08
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	8	1.08
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	8	1.08
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	8	1.08
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	8	1.08
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	8	1.08
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	8	1.08
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	8	1.08
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	8	1.08
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	8	1.08
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	5	1.08
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	5	1.08
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	5	1.08
(1,709)	1:118:B:VAL:HG21	1:123:B:PHE:H	16	1.08
(1,709)	1:118:B:VAL:HG22	1:123:B:PHE:H	16	1.08
(1,709)	1:118:B:VAL:HG23	1:123:B:PHE:H	16	1.08
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	20	1.07
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG21	20	1.07
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG22	20	1.07
(1,1081)	1:117:C:MET:H	1:118:C:VAL:HG23	20	1.07
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	19	1.07
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	19	1.07
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	19	1.07
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	19	1.07
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	19	1.07
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	19	1.07
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	19	1.07
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	19	1.07
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	19	1.07
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	2	1.07
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	2	1.07
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	2	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	2	1.07
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	2	1.07
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	2	1.07
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	2	1.07
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	2	1.07
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	2	1.07
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	18	1.07
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	18	1.07
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	18	1.07
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	9	1.06
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	9	1.06
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	9	1.06
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	9	1.06
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	9	1.06
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	9	1.06
(1,1098)	1:126:C:LEU:HD11	1:127:C:ASN:H	20	1.06
(1,1098)	1:126:C:LEU:HD12	1:127:C:ASN:H	20	1.06
(1,1098)	1:126:C:LEU:HD13	1:127:C:ASN:H	20	1.06
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	5	1.06
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	5	1.06
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	5	1.06
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	17	1.06
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	17	1.06
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	17	1.06
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	13	1.05
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	5	1.05
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	9	1.05
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	15	1.05
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	7	1.05
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	7	1.05
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	7	1.05
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	9	1.05
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	9	1.05
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	9	1.05
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	16	1.05
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	16	1.05
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	16	1.05
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	2	1.05
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	2	1.05
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	2	1.05
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	14	1.05
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	14	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	14	1.05
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	1	1.05
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	7	1.05
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	14	1.04
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	14	1.04
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	14	1.04
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	11	1.04
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD21	16	1.04
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD22	16	1.04
(1,1193)	1:31:D:VAL:HG11	1:68:D:LEU:HD23	16	1.04
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD21	16	1.04
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD22	16	1.04
(1,1193)	1:31:D:VAL:HG12	1:68:D:LEU:HD23	16	1.04
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD21	16	1.04
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD22	16	1.04
(1,1193)	1:31:D:VAL:HG13	1:68:D:LEU:HD23	16	1.04
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE1	7	1.04
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE2	7	1.04
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE3	7	1.04
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE1	7	1.04
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE2	7	1.04
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE3	7	1.04
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	20	1.04
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	20	1.04
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	20	1.04
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	20	1.04
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	20	1.04
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	20	1.04
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	10	1.03
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	10	1.03
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	10	1.03
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	1	1.03
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	1	1.03
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	1	1.03
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	1	1.03
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	1	1.03
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	1	1.03
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	1	1.03
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	1	1.03
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	1	1.03
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	9	1.03
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	9	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	9	1.03
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	9	1.03
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	9	1.03
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	9	1.03
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	9	1.03
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	9	1.03
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	9	1.03
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	17	1.03
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	17	1.03
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	17	1.03
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	4	1.02
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	1	1.02
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	1	1.02
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	1	1.02
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	1	1.02
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	1	1.02
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	1	1.02
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	1	1.02
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	13	1.02
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	13	1.02
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	13	1.02
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	3	1.02
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	17	1.01
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	17	1.01
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	17	1.01
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	17	1.01
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	17	1.01
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	17	1.01
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	17	1.01
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	17	1.01
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	17	1.01
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	15	1.01
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	12	1.01
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	19	1.01
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	19	1.01
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	19	1.01
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	18	1.01
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	18	1.01
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	18	1.01
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	6	1.01
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	6	1.01
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	6	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	6	1.01
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	6	1.01
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	6	1.01
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	6	1.01
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	6	1.01
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	6	1.01
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	3	1.0
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	3	1.0
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	3	1.0
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	19	1.0
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	18	1.0
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	18	1.0
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	18	1.0
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	3	1.0
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	3	1.0
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	3	1.0
(1,941)	1:60:C:LEU:HD11	1:61:C:ARG:H	14	1.0
(1,941)	1:60:C:LEU:HD12	1:61:C:ARG:H	14	1.0
(1,941)	1:60:C:LEU:HD13	1:61:C:ARG:H	14	1.0
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	2	1.0
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	2	1.0
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	2	1.0
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	15	1.0
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	13	1.0
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	13	1.0
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	13	1.0
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	20	1.0
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	20	1.0
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	20	1.0
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG21	13	0.99
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG22	13	0.99
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG23	13	0.99
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG21	13	0.99
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG22	13	0.99
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG23	13	0.99
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG21	13	0.99
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG22	13	0.99
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG23	13	0.99
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	16	0.99
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	3	0.99
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	3	0.99
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	3	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	3	0.99
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	3	0.99
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	3	0.99
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	3	0.99
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	3	0.99
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	3	0.99
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	6	0.99
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	6	0.99
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	6	0.99
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	6	0.99
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	6	0.99
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	6	0.99
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	6	0.99
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	6	0.99
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	6	0.99
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	9	0.99
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	9	0.99
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	9	0.99
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	9	0.99
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	9	0.99
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	9	0.99
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	9	0.99
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	9	0.99
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	9	0.99
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	15	0.99
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	15	0.99
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	15	0.99
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG21	4	0.99
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG22	4	0.99
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG23	4	0.99
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG21	4	0.99
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG22	4	0.99
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG23	4	0.99
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG21	4	0.99
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG22	4	0.99
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG23	4	0.99
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	3	0.99
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	3	0.99
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	3	0.99
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	3	0.99
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	3	0.99
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	3	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	3	0.99
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	3	0.99
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	3	0.99
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	15	0.99
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	15	0.99
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	15	0.99
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	9	0.99
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	9	0.99
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	9	0.99
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	13	0.98
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	13	0.98
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	13	0.98
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	13	0.98
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	13	0.98
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	13	0.98
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	13	0.98
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	13	0.98
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	13	0.98
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	19	0.98
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	3	0.98
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	3	0.98
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	3	0.98
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	3	0.98
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	3	0.98
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	3	0.98
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	3	0.98
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	3	0.98
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	3	0.98
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	6	0.98
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	8	0.98
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	8	0.98
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	8	0.98
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	6	0.98
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	6	0.98
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	6	0.98
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	16	0.98
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	16	0.98
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	16	0.98
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	16	0.98
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	16	0.98
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	16	0.98
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	16	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	16	0.98
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	16	0.98
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	6	0.98
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	6	0.98
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	6	0.98
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	4	0.98
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	4	0.98
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	4	0.98
(1,94)	1:36:A:TRP:HE3	1:37:A:GLN:H	10	0.98
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	19	0.98
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	3	0.97
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	3	0.97
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	3	0.97
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	3	0.97
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	3	0.97
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	3	0.97
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	7	0.97
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	10	0.97
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	10	0.97
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	10	0.97
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	1	0.97
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	10	0.97
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	10	0.97
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	10	0.97
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	12	0.97
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	12	0.97
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	12	0.97
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	12	0.97
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	12	0.97
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	12	0.97
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	12	0.97
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	12	0.97
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	12	0.97
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	2	0.97
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	2	0.97
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	2	0.97
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	2	0.97
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	2	0.97
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	2	0.97
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	2	0.97
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	2	0.97
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	2	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	2	0.97
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	2	0.97
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	2	0.97
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	2	0.97
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	2	0.97
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	2	0.97
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	2	0.97
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	2	0.97
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	2	0.97
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	3	0.97
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	3	0.97
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	3	0.97
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	16	0.96
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	16	0.96
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	16	0.96
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	12	0.96
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	12	0.96
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	12	0.96
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	12	0.96
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	12	0.96
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	12	0.96
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	12	0.96
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	12	0.96
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	12	0.96
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	18	0.96
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	15	0.96
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	15	0.96
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	15	0.96
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	17	0.96
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	17	0.96
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	17	0.96
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	2	0.96
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	2	0.96
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	2	0.96
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	7	0.96
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	7	0.96
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	7	0.96
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	15	0.96
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	15	0.96
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	15	0.96
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	13	0.96
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	13	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	13	0.96
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	13	0.96
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	13	0.96
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	13	0.96
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	14	0.96
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	14	0.96
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	14	0.96
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	14	0.96
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	14	0.96
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	14	0.96
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	14	0.96
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	14	0.96
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	14	0.96
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD1	7	0.96
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD2	7	0.96
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	2	0.96
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	10	0.96
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	18	0.96
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	7	0.95
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	7	0.95
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	7	0.95
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	7	0.95
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	7	0.95
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	7	0.95
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	7	0.95
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	7	0.95
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	7	0.95
(1,1215)	1:39:D:GLU:H	1:67:D:SER:H	20	0.95
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	16	0.95
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	8	0.95
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	13	0.95
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	2	0.95
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	2	0.95
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	2	0.95
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	18	0.95
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	18	0.95
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	18	0.95
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD11	18	0.95
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD12	18	0.95
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD13	18	0.95
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD11	18	0.95
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD12	18	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD13	18	0.95
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD11	18	0.95
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD12	18	0.95
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD13	18	0.95
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	1	0.95
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	7	0.95
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	7	0.95
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	7	0.95
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	7	0.95
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	7	0.95
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	7	0.95
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	7	0.95
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	7	0.95
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	7	0.95
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	3	0.95
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	15	0.94
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	15	0.94
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	15	0.94
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	15	0.94
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	17	0.94
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	5	0.94
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	5	0.94
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	5	0.94
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	9	0.94
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	9	0.93
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	9	0.93
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	9	0.93
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	15	0.93
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	17	0.93
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	17	0.93
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	17	0.93
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	8	0.93
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	8	0.93
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	8	0.93
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	19	0.93
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	19	0.93
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	19	0.93
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	20	0.93
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	20	0.93
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	20	0.93
(1,872)	1:44:C:LEU:HD11	1:63:C:THR:H	9	0.93
(1,872)	1:44:C:LEU:HD12	1:63:C:THR:H	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,872)	1:44:C:LEU:HD13	1:63:C:THR:H	9	0.93
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	17	0.93
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	17	0.93
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	17	0.93
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	17	0.93
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	17	0.93
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	17	0.93
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	17	0.93
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	17	0.93
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	17	0.93
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	4	0.93
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	4	0.93
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	4	0.93
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	11	0.93
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	11	0.93
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	11	0.93
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	11	0.93
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	11	0.93
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	11	0.93
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	11	0.93
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	11	0.93
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	11	0.93
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG21	5	0.92
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG22	5	0.92
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG23	5	0.92
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG21	5	0.92
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG22	5	0.92
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG23	5	0.92
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG21	5	0.92
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG22	5	0.92
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG23	5	0.92
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	1	0.92
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	1	0.92
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	1	0.92
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	1	0.92
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	1	0.92
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	1	0.92
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	1	0.92
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	1	0.92
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	1	0.92
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	13	0.92
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	13	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	13	0.92
(1,872)	1:44:C:LEU:HD11	1:63:C:THR:H	14	0.92
(1,872)	1:44:C:LEU:HD12	1:63:C:THR:H	14	0.92
(1,872)	1:44:C:LEU:HD13	1:63:C:THR:H	14	0.92
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	7	0.92
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	7	0.92
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	7	0.92
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	13	0.92
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	13	0.92
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	13	0.92
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	13	0.92
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	13	0.92
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	13	0.92
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	5	0.91
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	5	0.91
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	5	0.91
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	17	0.91
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	20	0.91
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	20	0.91
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	20	0.91
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	20	0.91
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	20	0.91
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	20	0.91
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	20	0.91
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	20	0.91
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	20	0.91
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	10	0.91
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	12	0.91
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	16	0.91
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	14	0.91
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	1	0.91
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	1	0.91
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	1	0.91
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	4	0.91
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	4	0.91
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	4	0.91
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	7	0.91
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	7	0.91
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	7	0.91
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	20	0.91
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	20	0.91
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	20	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	20	0.91
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	20	0.91
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	20	0.91
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	20	0.91
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	20	0.91
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	20	0.91
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	13	0.91
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	13	0.91
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	13	0.91
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	15	0.91
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	16	0.91
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	16	0.91
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	16	0.91
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	5	0.91
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	5	0.91
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	5	0.91
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	4	0.91
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	11	0.91
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	19	0.9
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	19	0.9
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	19	0.9
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	19	0.9
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	19	0.9
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	19	0.9
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	6	0.9
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	6	0.9
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	6	0.9
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	9	0.9
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	9	0.9
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	9	0.9
(1,957)	1:64:C:VAL:HG21	1:128:C:LEU:HD21	16	0.9
(1,957)	1:64:C:VAL:HG21	1:128:C:LEU:HD22	16	0.9
(1,957)	1:64:C:VAL:HG21	1:128:C:LEU:HD23	16	0.9
(1,957)	1:64:C:VAL:HG22	1:128:C:LEU:HD21	16	0.9
(1,957)	1:64:C:VAL:HG22	1:128:C:LEU:HD22	16	0.9
(1,957)	1:64:C:VAL:HG22	1:128:C:LEU:HD23	16	0.9
(1,957)	1:64:C:VAL:HG23	1:128:C:LEU:HD21	16	0.9
(1,957)	1:64:C:VAL:HG23	1:128:C:LEU:HD22	16	0.9
(1,957)	1:64:C:VAL:HG23	1:128:C:LEU:HD23	16	0.9
(1,828)	1:31:C:VAL:HG21	1:36:C:TRP:HE3	15	0.9
(1,828)	1:31:C:VAL:HG22	1:36:C:TRP:HE3	15	0.9
(1,828)	1:31:C:VAL:HG23	1:36:C:TRP:HE3	15	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	15	0.9
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	15	0.9
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	15	0.9
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	6	0.89
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	13	0.89
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	13	0.89
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	13	0.89
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	13	0.89
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	13	0.89
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	13	0.89
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	13	0.89
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	13	0.89
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	13	0.89
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	13	0.89
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	6	0.89
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	6	0.89
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	6	0.89
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	2	0.89
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	2	0.89
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	2	0.89
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	14	0.89
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	14	0.89
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	14	0.89
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG11	10	0.89
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG12	10	0.89
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG13	10	0.89
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG11	10	0.89
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG12	10	0.89
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG13	10	0.89
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG11	10	0.89
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG12	10	0.89
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG13	10	0.89
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	4	0.89
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	4	0.89
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	4	0.89
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	4	0.89
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	4	0.89
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	4	0.89
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	4	0.89
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	4	0.89
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	4	0.89
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	3	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	12	0.88
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	12	0.88
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	12	0.88
(1,1086)	1:118:C:VAL:HG21	1:119:C:SER:H	16	0.88
(1,1086)	1:118:C:VAL:HG22	1:119:C:SER:H	16	0.88
(1,1086)	1:118:C:VAL:HG23	1:119:C:SER:H	16	0.88
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	2	0.88
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	2	0.88
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	2	0.88
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	19	0.88
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	19	0.88
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	19	0.88
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	19	0.88
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	19	0.88
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	19	0.88
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	19	0.88
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	19	0.88
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	19	0.88
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	17	0.88
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	7	0.88
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	5	0.88
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	13	0.87
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	16	0.87
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	5	0.87
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	5	0.87
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	5	0.87
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	5	0.87
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	15	0.87
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	15	0.87
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	15	0.87
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	1	0.87
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	1	0.87
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	1	0.87
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	18	0.87
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	5	0.87
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	9	0.87
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	4	0.86
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	10	0.86
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	10	0.86
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	10	0.86
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	17	0.86
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	17	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	17	0.86
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD11	20	0.86
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD12	20	0.86
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD13	20	0.86
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD11	20	0.86
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD12	20	0.86
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD13	20	0.86
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD11	20	0.86
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD12	20	0.86
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD13	20	0.86
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	15	0.86
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	15	0.86
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	15	0.86
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	15	0.86
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	15	0.86
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	15	0.86
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	15	0.86
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	15	0.86
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	15	0.86
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	19	0.86
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	19	0.86
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	19	0.86
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	19	0.86
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	19	0.86
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	19	0.86
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	19	0.86
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	19	0.86
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	19	0.86
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	8	0.86
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	8	0.86
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	8	0.86
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	14	0.86
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	10	0.85
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	20	0.85
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	20	0.85
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	20	0.85
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	20	0.85
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	20	0.85
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	20	0.85
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	20	0.85
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	20	0.85
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	20	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	19	0.85
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	19	0.85
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	19	0.85
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	20	0.85
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	20	0.85
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	20	0.85
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	7	0.85
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	17	0.85
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	17	0.85
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	2	0.85
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	9	0.85
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG21	12	0.85
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG22	12	0.85
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG23	12	0.85
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG21	12	0.85
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG22	12	0.85
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG23	12	0.85
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG21	12	0.85
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG22	12	0.85
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG23	12	0.85
(1,194)	1:60:A:LEU:HD11	1:61:A:ARG:H	9	0.85
(1,194)	1:60:A:LEU:HD12	1:61:A:ARG:H	9	0.85
(1,194)	1:60:A:LEU:HD13	1:61:A:ARG:H	9	0.85
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	13	0.85
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	13	0.85
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	13	0.85
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	9	0.84
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	2	0.84
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB1	3	0.84
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB2	3	0.84
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB3	3	0.84
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB1	3	0.84
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB2	3	0.84
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB3	3	0.84
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB1	3	0.84
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB2	3	0.84
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB3	3	0.84
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	16	0.84
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	16	0.84
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	16	0.84
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	1	0.84
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	12	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	12	0.84
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	12	0.84
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	17	0.84
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	17	0.84
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	17	0.84
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG21	12	0.84
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG22	12	0.84
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG23	12	0.84
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG21	12	0.84
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG22	12	0.84
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG23	12	0.84
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG21	12	0.84
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG22	12	0.84
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG23	12	0.84
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	4	0.84
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	4	0.84
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	4	0.84
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	14	0.83
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	15	0.83
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	15	0.83
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	15	0.83
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	6	0.83
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	9	0.83
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	9	0.83
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	9	0.83
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	9	0.83
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	9	0.83
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	9	0.83
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	9	0.83
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	9	0.83
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	9	0.83
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	15	0.83
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	15	0.83
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	15	0.83
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	15	0.83
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	15	0.83
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	15	0.83
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	15	0.83
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	15	0.83
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	15	0.83
(1,115)	1:42:A:LEU:HD21	1:43:A:ASP:H	7	0.83
(1,115)	1:42:A:LEU:HD22	1:43:A:ASP:H	7	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:42:A:LEU:HD23	1:43:A:ASP:H	7	0.83
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	17	0.83
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	17	0.83
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	17	0.83
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	17	0.83
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	17	0.83
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	17	0.83
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	17	0.83
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	17	0.83
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	17	0.83
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	3	0.83
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	3	0.83
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	3	0.83
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	2	0.82
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	2	0.82
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	2	0.82
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	5	0.82
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	5	0.82
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	5	0.82
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	5	0.82
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	5	0.82
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	5	0.82
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	5	0.82
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	5	0.82
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	5	0.82
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	18	0.82
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	18	0.82
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	18	0.82
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	18	0.82
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	18	0.82
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	18	0.82
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	14	0.82
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	14	0.82
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	14	0.82
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	1	0.82
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	19	0.82
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	19	0.82
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	19	0.82
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	17	0.82
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	16	0.82
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	18	0.82
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	18	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	18	0.82
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	18	0.82
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	18	0.82
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	18	0.82
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	20	0.82
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	12	0.82
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	20	0.82
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	10	0.82
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	10	0.82
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	10	0.82
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	10	0.82
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	7	0.82
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	17	0.82
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	10	0.81
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	13	0.81
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	18	0.81
(1,824)	1:31:C:VAL:HG11	1:32:C:PHE:H	16	0.81
(1,824)	1:31:C:VAL:HG12	1:32:C:PHE:H	16	0.81
(1,824)	1:31:C:VAL:HG13	1:32:C:PHE:H	16	0.81
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	5	0.81
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	5	0.81
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	5	0.81
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	16	0.81
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	16	0.81
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	16	0.81
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	2	0.81
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	2	0.81
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	2	0.81
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	2	0.81
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	2	0.81
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	2	0.81
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	2	0.81
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	2	0.81
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	2	0.81
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	4	0.81
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	4	0.81
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	8	0.81
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	20	0.81
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	17	0.81
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	13	0.81
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	12	0.8
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	19	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	19	0.8
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	19	0.8
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	19	0.8
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	19	0.8
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	19	0.8
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	19	0.8
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	19	0.8
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	19	0.8
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	14	0.8
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	13	0.8
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	13	0.8
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	13	0.8
(1,1292)	1:60:D:LEU:HD11	1:62:D:VAL:H	12	0.8
(1,1292)	1:60:D:LEU:HD12	1:62:D:VAL:H	12	0.8
(1,1292)	1:60:D:LEU:HD13	1:62:D:VAL:H	12	0.8
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	18	0.8
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	3	0.8
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	4	0.8
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	4	0.8
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	4	0.8
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	4	0.8
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	4	0.8
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	4	0.8
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	4	0.8
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	4	0.8
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	4	0.8
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	20	0.8
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	13	0.8
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	13	0.8
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	13	0.8
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	13	0.8
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	13	0.8
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	13	0.8
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	13	0.8
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	13	0.8
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	13	0.8
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	10	0.8
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	10	0.8
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	10	0.8
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	10	0.8
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	10	0.8
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	10	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	10	0.8
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	10	0.8
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	10	0.8
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	10	0.8
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	7	0.8
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	14	0.8
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	16	0.8
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	17	0.8
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	18	0.8
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	18	0.8
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	18	0.8
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	15	0.8
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	4	0.79
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	4	0.79
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	4	0.79
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	16	0.79
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	5	0.79
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	5	0.79
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	5	0.79
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	2	0.79
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	3	0.79
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	18	0.79
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	18	0.79
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	18	0.79
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	18	0.79
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	18	0.79
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	18	0.79
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	18	0.79
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	18	0.79
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	18	0.79
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	20	0.79
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	20	0.79
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	20	0.79
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	7	0.79
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	8	0.79
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	8	0.79
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	8	0.79
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	8	0.79
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	8	0.79
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	8	0.79
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	17	0.79
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	19	0.79
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	19	0.79
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	19	0.79
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	19	0.79
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	13	0.79
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	13	0.79
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	13	0.79
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	13	0.78
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	13	0.78
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	13	0.78
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	14	0.78
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	14	0.78
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	14	0.78
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	14	0.78
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	14	0.78
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	14	0.78
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	14	0.78
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	14	0.78
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	14	0.78
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	8	0.78
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	8	0.78
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	8	0.78
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD21	13	0.78
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD22	13	0.78
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD23	13	0.78
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD21	13	0.78
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD22	13	0.78
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD23	13	0.78
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD21	13	0.78
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD22	13	0.78
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD23	13	0.78
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	3	0.78
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	3	0.78
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	3	0.78
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	3	0.78
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	8	0.78
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	20	0.78
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	20	0.78
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	20	0.78
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	20	0.78
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	20	0.78
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	20	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	20	0.78
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	20	0.78
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	20	0.78
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	15	0.78
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	15	0.78
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	15	0.78
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	4	0.78
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	17	0.78
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	17	0.78
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	17	0.78
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	10	0.78
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	17	0.78
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	18	0.78
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	5	0.78
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	3	0.77
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	3	0.77
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	3	0.77
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	3	0.77
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	17	0.77
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	17	0.77
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	17	0.77
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	17	0.77
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	17	0.77
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	17	0.77
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	17	0.77
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	17	0.77
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	17	0.77
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	16	0.77
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	3	0.77
(1,1046)	1:98:C:LEU:HD11	1:99:C:GLY:H	3	0.77
(1,1046)	1:98:C:LEU:HD12	1:99:C:GLY:H	3	0.77
(1,1046)	1:98:C:LEU:HD13	1:99:C:GLY:H	3	0.77
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE1	5	0.77
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE2	5	0.77
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE3	5	0.77
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE1	5	0.77
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE2	5	0.77
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE3	5	0.77
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	10	0.77
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	12	0.77
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	9	0.77
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	16	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	16	0.77
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	16	0.77
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	16	0.77
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	18	0.77
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	18	0.77
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	18	0.77
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	1	0.77
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	13	0.77
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	2	0.77
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	6	0.77
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	1	0.77
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	1	0.77
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	1	0.77
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	1	0.77
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	1	0.77
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	1	0.77
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	1	0.77
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	1	0.77
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	1	0.77
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	17	0.77
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	17	0.77
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	17	0.77
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	7	0.77
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	7	0.77
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	7	0.77
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	8	0.77
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	8	0.77
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	8	0.77
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	2	0.76
(1,1292)	1:60:D:LEU:HD11	1:62:D:VAL:H	3	0.76
(1,1292)	1:60:D:LEU:HD12	1:62:D:VAL:H	3	0.76
(1,1292)	1:60:D:LEU:HD13	1:62:D:VAL:H	3	0.76
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	12	0.76
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	12	0.76
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	12	0.76
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	12	0.76
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	12	0.76
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	12	0.76
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	12	0.76
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	12	0.76
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	12	0.76
(1,1225)	1:42:D:LEU:HD21	1:43:D:ASP:H	6	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:42:D:LEU:HD22	1:43:D:ASP:H	6	0.76
(1,1225)	1:42:D:LEU:HD23	1:43:D:ASP:H	6	0.76
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	5	0.76
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	5	0.76
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	5	0.76
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	1	0.76
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	7	0.76
(1,824)	1:31:C:VAL:HG11	1:32:C:PHE:H	5	0.76
(1,824)	1:31:C:VAL:HG12	1:32:C:PHE:H	5	0.76
(1,824)	1:31:C:VAL:HG13	1:32:C:PHE:H	5	0.76
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	3	0.76
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	3	0.76
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	3	0.76
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	8	0.76
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	8	0.76
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	8	0.76
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	14	0.76
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	14	0.76
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	14	0.76
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	14	0.76
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	14	0.76
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	14	0.76
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	14	0.76
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	14	0.76
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	14	0.76
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	13	0.76
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	14	0.76
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	14	0.76
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	14	0.76
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	17	0.76
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	6	0.76
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	20	0.76
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	5	0.75
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	2	0.75
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	6	0.75
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	6	0.75
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	6	0.75
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	18	0.75
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	18	0.75
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	18	0.75
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	15	0.75
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	15	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	15	0.75
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	15	0.75
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	15	0.75
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	15	0.75
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	15	0.75
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	15	0.75
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	15	0.75
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	3	0.75
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	13	0.75
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	13	0.75
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	13	0.75
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	1	0.75
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	1	0.75
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	1	0.75
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	15	0.75
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	8	0.75
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	8	0.75
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	8	0.75
(1,403)	1:9:B:MET:HE1	1:10:B:THR:H	15	0.75
(1,403)	1:9:B:MET:HE2	1:10:B:THR:H	15	0.75
(1,403)	1:9:B:MET:HE3	1:10:B:THR:H	15	0.75
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	3	0.75
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	3	0.75
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	3	0.75
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	3	0.75
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	3	0.75
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	3	0.75
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	20	0.75
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	20	0.75
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	20	0.75
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	7	0.75
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	6	0.75
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	6	0.75
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	6	0.75
(1,94)	1:36:A:TRP:HE3	1:37:A:GLN:H	13	0.75
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	1	0.75
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	6	0.74
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	6	0.74
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	6	0.74
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	6	0.74
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	6	0.74
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	6	0.74
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	6	0.74
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	6	0.74
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	10	0.74
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	10	0.74
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	10	0.74
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	4	0.74
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	12	0.74
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	19	0.74
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	19	0.74
(1,1130)	1:140:C:TYR:HD1	1:141:C:LEU:H	17	0.74
(1,1130)	1:140:C:TYR:HD2	1:141:C:LEU:H	17	0.74
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	4	0.74
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	4	0.74
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	4	0.74
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	8	0.74
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	8	0.74
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	8	0.74
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	2	0.74
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	2	0.74
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	2	0.74
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	2	0.74
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	2	0.74
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	2	0.74
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	2	0.74
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	2	0.74
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	2	0.74
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	18	0.74
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	18	0.74
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	18	0.74
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	12	0.74
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	19	0.74
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	16	0.74
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	16	0.74
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	16	0.74
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	16	0.74
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	16	0.74
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	16	0.74
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	10	0.74
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	18	0.74
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	13	0.74
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	13	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	13	0.74
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	13	0.74
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	13	0.74
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	13	0.74
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	13	0.74
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	13	0.74
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	13	0.74
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE1	20	0.74
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE2	20	0.74
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE1	20	0.74
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE2	20	0.74
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE1	20	0.74
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE2	20	0.74
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	18	0.73
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	15	0.73
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	15	0.73
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	15	0.73
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	15	0.73
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	15	0.73
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	15	0.73
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	15	0.73
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	15	0.73
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	15	0.73
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	3	0.73
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	3	0.73
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	3	0.73
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	18	0.73
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	6	0.73
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	20	0.73
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	3	0.73
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	3	0.73
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	3	0.73
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD21	19	0.73
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD22	19	0.73
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD23	19	0.73
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	17	0.73
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	17	0.73
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	17	0.73
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	8	0.73
(1,468)	1:34:B:LYS:H	1:35:B:ASP:H	16	0.73
(1,403)	1:9:B:MET:HE1	1:10:B:THR:H	19	0.73
(1,403)	1:9:B:MET:HE2	1:10:B:THR:H	19	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:9:B:MET:HE3	1:10:B:THR:H	19	0.73
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	14	0.73
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	8	0.73
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	18	0.73
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	19	0.73
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	6	0.73
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	6	0.73
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	6	0.73
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	5	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	5	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	5	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	5	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	5	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	5	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	5	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	5	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	5	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	9	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	9	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	9	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	9	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	9	0.72
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	9	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	9	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	9	0.72
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	9	0.72
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	20	0.72
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	1	0.72
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	14	0.72
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	14	0.72
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	14	0.72
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	1	0.72
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	1	0.72
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	1	0.72
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	5	0.72
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	7	0.72
(1,403)	1:9:B:MET:HE1	1:10:B:THR:H	6	0.72
(1,403)	1:9:B:MET:HE2	1:10:B:THR:H	6	0.72
(1,403)	1:9:B:MET:HE3	1:10:B:THR:H	6	0.72
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	9	0.72
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	4	0.72
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	4	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	4	0.72
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	4	0.72
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	4	0.72
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	4	0.72
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	16	0.72
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	19	0.72
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	19	0.72
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	19	0.72
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	8	0.72
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	8	0.72
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	8	0.72
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	14	0.72
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	14	0.72
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	4	0.71
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	4	0.71
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	4	0.71
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	4	0.71
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	4	0.71
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	4	0.71
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	4	0.71
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	4	0.71
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	4	0.71
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	8	0.71
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	3	0.71
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	3	0.71
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	3	0.71
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	19	0.71
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	19	0.71
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	19	0.71
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	5	0.71
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	11	0.71
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	13	0.71
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	19	0.71
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG11	10	0.71
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG12	10	0.71
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG13	10	0.71
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG11	10	0.71
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG12	10	0.71
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG13	10	0.71
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG11	10	0.71
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG12	10	0.71
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG13	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB1	6	0.71
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB2	6	0.71
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB3	6	0.71
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	20	0.71
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	20	0.71
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	20	0.71
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	18	0.71
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	1	0.71
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	2	0.71
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	2	0.71
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	2	0.71
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	9	0.71
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	9	0.71
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	9	0.71
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	9	0.71
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	9	0.71
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	9	0.71
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	9	0.71
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	9	0.71
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	9	0.71
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	1	0.71
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	1	0.71
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	1	0.71
(1,78)	1:31:A:VAL:HG11	1:123:A:PHE:HE1	7	0.71
(1,78)	1:31:A:VAL:HG11	1:123:A:PHE:HE2	7	0.71
(1,78)	1:31:A:VAL:HG12	1:123:A:PHE:HE1	7	0.71
(1,78)	1:31:A:VAL:HG12	1:123:A:PHE:HE2	7	0.71
(1,78)	1:31:A:VAL:HG13	1:123:A:PHE:HE1	7	0.71
(1,78)	1:31:A:VAL:HG13	1:123:A:PHE:HE2	7	0.71
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	14	0.71
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	14	0.71
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	16	0.7
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	16	0.7
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	16	0.7
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	7	0.7
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	7	0.7
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	7	0.7
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	7	0.7
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	7	0.7
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	7	0.7
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	7	0.7
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	7	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	7	0.7
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	18	0.7
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	18	0.7
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	18	0.7
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	18	0.7
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	18	0.7
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	18	0.7
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	18	0.7
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	18	0.7
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	18	0.7
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	13	0.7
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	13	0.7
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	13	0.7
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	10	0.7
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	10	0.7
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	10	0.7
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	18	0.7
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	7	0.7
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	4	0.7
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	20	0.7
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	20	0.7
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	8	0.7
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	8	0.7
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	8	0.7
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	18	0.7
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	18	0.7
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	18	0.7
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	16	0.7
(1,403)	1:9:B:MET:HE1	1:10:B:THR:H	10	0.7
(1,403)	1:9:B:MET:HE2	1:10:B:THR:H	10	0.7
(1,403)	1:9:B:MET:HE3	1:10:B:THR:H	10	0.7
(1,368)	1:128:A:LEU:HD11	1:129:A:ALA:H	11	0.7
(1,368)	1:128:A:LEU:HD12	1:129:A:ALA:H	11	0.7
(1,368)	1:128:A:LEU:HD13	1:129:A:ALA:H	11	0.7
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	19	0.7
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	19	0.7
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	19	0.7
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	13	0.7
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	13	0.7
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	13	0.7
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	2	0.7
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	11	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD21	15	0.69
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD22	15	0.69
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD23	15	0.69
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD21	15	0.69
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD22	15	0.69
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD23	15	0.69
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD21	15	0.69
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD22	15	0.69
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD23	15	0.69
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	8	0.69
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	8	0.69
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	8	0.69
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	17	0.69
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	17	0.69
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	17	0.69
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	1	0.69
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	13	0.69
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	13	0.69
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	13	0.69
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	18	0.69
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	18	0.69
(1,492)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	18	0.69
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	18	0.69
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	18	0.69
(1,492)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	18	0.69
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	18	0.69
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	18	0.69
(1,492)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	18	0.69
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	9	0.69
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	14	0.69
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	3	0.69
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	4	0.69
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	14	0.69
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	14	0.69
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	14	0.69
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	18	0.68
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	18	0.68
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	18	0.68
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	18	0.68
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	18	0.68
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	18	0.68
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	18	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	18	0.68
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	18	0.68
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	2	0.68
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	9	0.68
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	9	0.68
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	9	0.68
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	1	0.68
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	14	0.68
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	3	0.68
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	3	0.68
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	3	0.68
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	3	0.68
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	9	0.68
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	1	0.68
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	1	0.68
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	1	0.68
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	1	0.68
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	1	0.68
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	1	0.68
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	15	0.68
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	15	0.68
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	15	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	1	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	1	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	1	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	6	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	6	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	6	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	12	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	12	0.68
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	12	0.68
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	3	0.68
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	1	0.68
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	18	0.68
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	18	0.68
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	18	0.68
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	18	0.68
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	18	0.68
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	18	0.68
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	18	0.68
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	18	0.68
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	18	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:34:B:LYS:H	1:35:B:ASP:H	17	0.68
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	9	0.68
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	17	0.68
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	14	0.68
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	14	0.68
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	14	0.68
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	5	0.68
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	5	0.68
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	5	0.68
(1,87)	1:32:A:PHE:HD1	1:36:A:TRP:HZ3	18	0.68
(1,87)	1:32:A:PHE:HD2	1:36:A:TRP:HZ3	18	0.68
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	8	0.68
(1,34)	1:19:A:LYS:H	1:79:A:GLN:H	16	0.68
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	16	0.67
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	16	0.67
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	16	0.67
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	3	0.67
(1,1208)	1:35:D:ASP:H	1:36:D:TRP:HZ3	8	0.67
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	5	0.67
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	5	0.67
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	10	0.67
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	10	0.67
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	10	0.67
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	9	0.67
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	14	0.67
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD21	9	0.67
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD22	9	0.67
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD23	9	0.67
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	12	0.67
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	12	0.67
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	12	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	4	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	4	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	4	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	10	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	10	0.67
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	10	0.67
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	12	0.67
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	12	0.67
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	12	0.67
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	12	0.67
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	12	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	12	0.67
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	12	0.67
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	12	0.67
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	12	0.67
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	1	0.67
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	1	0.67
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	1	0.67
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	15	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG21	1	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG22	1	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG23	1	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG21	1	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG22	1	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG23	1	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG21	1	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG22	1	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG23	1	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG21	6	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG22	6	0.67
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG23	6	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG21	6	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG22	6	0.67
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG23	6	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG21	6	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG22	6	0.67
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG23	6	0.67
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	16	0.67
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	16	0.67
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	16	0.67
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	16	0.67
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	16	0.67
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	16	0.67
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	16	0.67
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	16	0.67
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	16	0.67
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	7	0.67
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	7	0.67
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	7	0.67
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	9	0.67
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	9	0.67
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	9	0.67
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	12	0.66
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	12	0.66
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	12	0.66
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	12	0.66
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	12	0.66
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	12	0.66
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	12	0.66
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	12	0.66
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD11	17	0.66
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD12	17	0.66
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD13	17	0.66
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD11	17	0.66
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD12	17	0.66
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD13	17	0.66
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD11	17	0.66
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD12	17	0.66
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD13	17	0.66
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	10	0.66
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	10	0.66
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	10	0.66
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	10	0.66
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	10	0.66
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	10	0.66
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	10	0.66
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	10	0.66
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	10	0.66
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	20	0.66
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	15	0.66
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	7	0.66
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	17	0.66
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	3	0.66
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	15	0.66
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	15	0.66
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	15	0.66
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	13	0.66
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	13	0.66
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD1	5	0.66
(1,740)	1:136:B:LEU:HD21	1:137:B:PHE:HD2	5	0.66
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD1	5	0.66
(1,740)	1:136:B:LEU:HD22	1:137:B:PHE:HD2	5	0.66
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD1	5	0.66
(1,740)	1:136:B:LEU:HD23	1:137:B:PHE:HD2	5	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	13	0.66
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	13	0.66
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	13	0.66
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	18	0.66
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	18	0.66
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	18	0.66
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	2	0.66
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	2	0.66
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	2	0.66
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	13	0.66
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	13	0.66
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	13	0.66
(1,468)	1:34:B:LYS:H	1:35:B:ASP:H	19	0.66
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	12	0.66
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	12	0.66
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	12	0.66
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	12	0.66
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	12	0.66
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	12	0.66
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	12	0.66
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	12	0.66
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	12	0.66
(1,233)	1:68:A:LEU:HD11	1:73:A:ALA:H	13	0.66
(1,233)	1:68:A:LEU:HD12	1:73:A:ALA:H	13	0.66
(1,233)	1:68:A:LEU:HD13	1:73:A:ALA:H	13	0.66
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	3	0.66
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	3	0.66
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	3	0.66
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	4	0.66
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	1	0.65
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	2	0.65
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	2	0.65
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	18	0.65
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	18	0.65
(1,1160)	1:19:D:LYS:H	1:79:D:GLN:H	10	0.65
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG21	3	0.65
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG22	3	0.65
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG23	3	0.65
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG21	3	0.65
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG22	3	0.65
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG23	3	0.65
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG21	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG22	3	0.65
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG23	3	0.65
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	20	0.65
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	16	0.65
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	3	0.65
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	3	0.65
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	3	0.65
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	3	0.65
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	3	0.65
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	3	0.65
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	3	0.65
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	3	0.65
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	3	0.65
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG11	17	0.65
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG12	17	0.65
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG13	17	0.65
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG11	17	0.65
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG12	17	0.65
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG13	17	0.65
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG11	17	0.65
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG12	17	0.65
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG13	17	0.65
(1,768)	1:14:C:GLN:H	1:85:C:SER:H	12	0.65
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	6	0.65
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	6	0.65
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	6	0.65
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	7	0.65
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	7	0.65
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	7	0.65
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	13	0.65
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	13	0.65
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	6	0.65
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	6	0.65
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	6	0.65
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	7	0.65
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	15	0.64
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	17	0.64
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	17	0.64
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	17	0.64
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD11	18	0.64
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD12	18	0.64
(1,1230)	1:43:D:ASP:H	1:44:D:LEU:HD13	18	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:42:D:LEU:HD21	1:43:D:ASP:H	20	0.64
(1,1225)	1:42:D:LEU:HD22	1:43:D:ASP:H	20	0.64
(1,1225)	1:42:D:LEU:HD23	1:43:D:ASP:H	20	0.64
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	16	0.64
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	16	0.64
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG21	16	0.64
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG22	16	0.64
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG23	16	0.64
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG21	16	0.64
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG22	16	0.64
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG23	16	0.64
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG21	16	0.64
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG22	16	0.64
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG23	16	0.64
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	6	0.64
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	6	0.64
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	6	0.64
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	5	0.64
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	7	0.64
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	10	0.64
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	10	0.64
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	10	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	3	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	3	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	3	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	9	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	9	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	9	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	19	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	19	0.64
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	19	0.64
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	16	0.64
(1,462)	1:31:B:VAL:HG21	1:123:B:PHE:HE1	19	0.64
(1,462)	1:31:B:VAL:HG21	1:123:B:PHE:HE2	19	0.64
(1,462)	1:31:B:VAL:HG22	1:123:B:PHE:HE1	19	0.64
(1,462)	1:31:B:VAL:HG22	1:123:B:PHE:HE2	19	0.64
(1,462)	1:31:B:VAL:HG23	1:123:B:PHE:HE1	19	0.64
(1,462)	1:31:B:VAL:HG23	1:123:B:PHE:HE2	19	0.64
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	13	0.64
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	13	0.64
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	13	0.64
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	13	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	13	0.64
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	13	0.64
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	13	0.64
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	13	0.64
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	13	0.64
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	5	0.64
(1,233)	1:68:A:LEU:HD11	1:73:A:ALA:H	19	0.64
(1,233)	1:68:A:LEU:HD12	1:73:A:ALA:H	19	0.64
(1,233)	1:68:A:LEU:HD13	1:73:A:ALA:H	19	0.64
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	5	0.64
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG11	10	0.64
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG12	10	0.64
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG13	10	0.64
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG11	10	0.64
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG12	10	0.64
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG13	10	0.64
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG11	10	0.64
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG12	10	0.64
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG13	10	0.64
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	12	0.64
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	1	0.63
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	7	0.63
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	7	0.63
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	12	0.63
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	17	0.63
(1,1110)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	17	0.63
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	17	0.63
(1,1110)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	17	0.63
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	17	0.63
(1,1110)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	17	0.63
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	3	0.63
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	3	0.63
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	3	0.63
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	8	0.63
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	8	0.63
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	8	0.63
(1,1087)	1:118:C:VAL:HG21	1:125:C:GLN:H	13	0.63
(1,1087)	1:118:C:VAL:HG22	1:125:C:GLN:H	13	0.63
(1,1087)	1:118:C:VAL:HG23	1:125:C:GLN:H	13	0.63
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	15	0.63
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	14	0.63
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	14	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	14	0.63
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	6	0.63
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	6	0.63
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	6	0.63
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	6	0.63
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	6	0.63
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	6	0.63
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	6	0.63
(1,297)	1:95:A:ALA:H	1:98:A:LEU:H	2	0.63
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	15	0.63
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	15	0.63
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	15	0.63
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	11	0.63
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	11	0.63
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	11	0.63
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	11	0.63
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	13	0.62
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	13	0.62
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	13	0.62
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	13	0.62
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	13	0.62
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	13	0.62
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	13	0.62
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	13	0.62
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	13	0.62
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	2	0.62
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	2	0.62
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	18	0.62
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	8	0.62
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	8	0.62
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	8	0.62
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	8	0.62
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	17	0.62
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	17	0.62
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	17	0.62
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	17	0.62
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	17	0.62
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	17	0.62
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	17	0.62
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	17	0.62
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	17	0.62
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	20	0.62
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	20	0.62
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	14	0.62
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	14	0.62
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	14	0.62
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	3	0.62
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	3	0.62
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	3	0.62
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	14	0.62
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	14	0.62
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	14	0.62
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	18	0.62
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	11	0.62
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	19	0.62
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	11	0.62
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	2	0.61
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	2	0.61
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	2	0.61
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	18	0.61
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	18	0.61
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	18	0.61
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	18	0.61
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	18	0.61
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	18	0.61
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	18	0.61
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	18	0.61
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	18	0.61
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	5	0.61
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	5	0.61
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	5	0.61
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	13	0.61
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	13	0.61
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	9	0.61
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD21	8	0.61
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD22	8	0.61
(1,933)	1:59:C:VAL:H	1:60:C:LEU:HD23	8	0.61
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG11	2	0.61
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG12	2	0.61
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG13	2	0.61
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	9	0.61
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	9	0.61
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	2	0.61
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	2	0.61
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	2	0.61
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	14	0.61
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	14	0.61
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	14	0.61
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	16	0.61
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	16	0.61
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	16	0.61
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	2	0.61
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	14	0.61
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	10	0.61
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	10	0.61
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	10	0.61
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	14	0.61
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	14	0.61
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	10	0.61
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	4	0.61
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	20	0.61
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	20	0.61
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	20	0.61
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	9	0.61
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	9	0.61
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	9	0.61
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	9	0.61
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	14	0.61
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	14	0.61
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	14	0.61
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	18	0.6
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	4	0.6
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	4	0.6
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	4	0.6
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	19	0.6
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	19	0.6
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	1	0.6
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	10	0.6
(1,872)	1:44:C:LEU:HD11	1:63:C:THR:H	3	0.6
(1,872)	1:44:C:LEU:HD12	1:63:C:THR:H	3	0.6
(1,872)	1:44:C:LEU:HD13	1:63:C:THR:H	3	0.6
(1,825)	1:31:C:VAL:HG11	1:32:C:PHE:HD1	16	0.6
(1,825)	1:31:C:VAL:HG11	1:32:C:PHE:HD2	16	0.6
(1,825)	1:31:C:VAL:HG12	1:32:C:PHE:HD1	16	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:31:C:VAL:HG12	1:32:C:PHE:HD2	16	0.6
(1,825)	1:31:C:VAL:HG13	1:32:C:PHE:HD1	16	0.6
(1,825)	1:31:C:VAL:HG13	1:32:C:PHE:HD2	16	0.6
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	19	0.6
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	19	0.6
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG11	17	0.6
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG12	17	0.6
(1,702)	1:117:B:MET:H	1:118:B:VAL:HG13	17	0.6
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	6	0.6
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	6	0.6
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	6	0.6
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	6	0.6
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	6	0.6
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	6	0.6
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	6	0.6
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	6	0.6
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	6	0.6
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	6	0.6
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	7	0.6
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	7	0.6
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	3	0.6
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	3	0.6
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	12	0.6
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	12	0.6
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	18	0.6
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	9	0.6
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	9	0.6
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	9	0.6
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	9	0.6
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	9	0.6
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	9	0.6
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	9	0.6
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	9	0.6
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	9	0.6
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	1	0.6
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	1	0.6
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	1	0.6
(1,1374)	1:87:D:ALA:H	1:89:D:ILE:H	1	0.59
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	17	0.59
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	17	0.59
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	17	0.59
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	17	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	17	0.59
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	17	0.59
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	17	0.59
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	17	0.59
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	17	0.59
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	15	0.59
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	15	0.59
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	15	0.59
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	13	0.59
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	13	0.59
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	11	0.59
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	11	0.59
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	17	0.59
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	17	0.59
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	17	0.59
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	17	0.59
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	12	0.59
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	7	0.59
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	7	0.59
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	7	0.59
(1,641)	1:92:B:THR:H	1:95:B:ALA:H	9	0.59
(1,630)	1:87:B:ALA:H	1:89:B:ILE:H	10	0.59
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	20	0.59
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	6	0.59
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	1	0.59
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	13	0.59
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	13	0.59
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	13	0.59
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	13	0.59
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	13	0.59
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	13	0.59
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	13	0.59
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	13	0.59
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	13	0.59
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	6	0.59
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	6	0.59
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	6	0.59
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	6	0.59
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	14	0.59
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	9	0.59
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	3	0.59
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	9	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	9	0.58
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	9	0.58
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	7	0.58
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	7	0.58
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	7	0.58
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	7	0.58
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	7	0.58
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	7	0.58
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	7	0.58
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	7	0.58
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	7	0.58
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	8	0.58
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	8	0.58
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	8	0.58
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	8	0.58
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	8	0.58
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	8	0.58
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	8	0.58
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	8	0.58
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	8	0.58
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	19	0.58
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	3	0.58
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	3	0.58
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	15	0.58
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	13	0.58
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	13	0.58
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	13	0.58
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	13	0.58
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	13	0.58
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	13	0.58
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	13	0.58
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	13	0.58
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	13	0.58
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	11	0.58
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	11	0.58
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	10	0.58
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	4	0.58
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	4	0.58
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	4	0.58
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	8	0.58
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	8	0.58
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	5	0.58
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	2	0.58
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	10	0.58
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	8	0.58
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	17	0.58
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	20	0.58
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	20	0.58
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	20	0.58
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	1	0.58
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	1	0.58
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	6	0.58
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	12	0.57
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	12	0.57
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	12	0.57
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	12	0.57
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	12	0.57
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	12	0.57
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	12	0.57
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	12	0.57
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	12	0.57
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	12	0.57
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	12	0.57
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	12	0.57
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	15	0.57
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	15	0.57
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	15	0.57
(1,1311)	1:64:D:VAL:HG21	1:126:D:LEU:HD21	18	0.57
(1,1311)	1:64:D:VAL:HG21	1:126:D:LEU:HD22	18	0.57
(1,1311)	1:64:D:VAL:HG21	1:126:D:LEU:HD23	18	0.57
(1,1311)	1:64:D:VAL:HG22	1:126:D:LEU:HD21	18	0.57
(1,1311)	1:64:D:VAL:HG22	1:126:D:LEU:HD22	18	0.57
(1,1311)	1:64:D:VAL:HG22	1:126:D:LEU:HD23	18	0.57
(1,1311)	1:64:D:VAL:HG23	1:126:D:LEU:HD21	18	0.57
(1,1311)	1:64:D:VAL:HG23	1:126:D:LEU:HD22	18	0.57
(1,1311)	1:64:D:VAL:HG23	1:126:D:LEU:HD23	18	0.57
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	12	0.57
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	12	0.57
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	12	0.57
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	12	0.57
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	12	0.57
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	12	0.57
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	11	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG21	15	0.57
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG22	15	0.57
(1,1106)	1:128:C:LEU:HD11	1:131:C:VAL:HG23	15	0.57
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG21	15	0.57
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG22	15	0.57
(1,1106)	1:128:C:LEU:HD12	1:131:C:VAL:HG23	15	0.57
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG21	15	0.57
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG22	15	0.57
(1,1106)	1:128:C:LEU:HD13	1:131:C:VAL:HG23	15	0.57
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	18	0.57
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	18	0.57
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	18	0.57
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	18	0.57
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	18	0.57
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	18	0.57
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	18	0.57
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	18	0.57
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	18	0.57
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	17	0.57
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	17	0.57
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	17	0.57
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	1	0.57
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	1	0.57
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	1	0.57
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	7	0.57
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	7	0.57
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	7	0.57
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	14	0.57
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	7	0.57
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	14	0.57
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	14	0.57
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	8	0.57
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	1	0.57
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	1	0.57
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	1	0.57
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	1	0.57
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	1	0.57
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	1	0.57
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG11	6	0.57
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG12	6	0.57
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG13	6	0.57
(1,120)	1:43:A:ASP:H	1:65:A:THR:H	19	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	8	0.56
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	6	0.56
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	6	0.56
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	6	0.56
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	6	0.56
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	6	0.56
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	6	0.56
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	6	0.56
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	6	0.56
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	6	0.56
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	6	0.56
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	17	0.56
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	17	0.56
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	17	0.56
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	12	0.56
(1,1046)	1:98:C:LEU:HD11	1:99:C:GLY:H	5	0.56
(1,1046)	1:98:C:LEU:HD12	1:99:C:GLY:H	5	0.56
(1,1046)	1:98:C:LEU:HD13	1:99:C:GLY:H	5	0.56
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	13	0.56
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	12	0.56
(1,824)	1:31:C:VAL:HG11	1:32:C:PHE:H	18	0.56
(1,824)	1:31:C:VAL:HG12	1:32:C:PHE:H	18	0.56
(1,824)	1:31:C:VAL:HG13	1:32:C:PHE:H	18	0.56
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	2	0.56
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	3	0.56
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	15	0.56
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	10	0.56
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	10	0.56
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	10	0.56
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	10	0.56
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	10	0.56
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	10	0.56
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	10	0.56
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	10	0.56
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	10	0.56
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	3	0.56
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	3	0.56
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	2	0.56
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	2	0.56
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	11	0.56
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	13	0.56
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	13	0.56
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	2	0.56
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	2	0.56
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	2	0.56
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	10	0.56
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	17	0.56
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	17	0.56
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	5	0.56
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	15	0.55
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG21	15	0.55
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG22	15	0.55
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG23	15	0.55
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG21	15	0.55
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG22	15	0.55
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG23	15	0.55
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG21	15	0.55
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG22	15	0.55
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG23	15	0.55
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	13	0.55
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	13	0.55
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	13	0.55
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	13	0.55
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	13	0.55
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	13	0.55
(1,1207)	1:35:D:ASP:H	1:36:D:TRP:HE1	16	0.55
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	14	0.55
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	14	0.55
(1,1108)	1:131:C:VAL:HG11	1:133:C:PHE:H	9	0.55
(1,1108)	1:131:C:VAL:HG12	1:133:C:PHE:H	9	0.55
(1,1108)	1:131:C:VAL:HG13	1:133:C:PHE:H	9	0.55
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	5	0.55
(1,1022)	1:91:C:GLY:H	1:95:C:ALA:H	17	0.55
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	11	0.55
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	6	0.55
(1,916)	1:56:C:TYR:HD1	1:86:C:ILE:H	18	0.55
(1,916)	1:56:C:TYR:HD2	1:86:C:ILE:H	18	0.55
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	15	0.55
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	15	0.55
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	15	0.55
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	15	0.55
(1,830)	1:31:C:VAL:HG21	1:123:C:PHE:HE1	9	0.55
(1,830)	1:31:C:VAL:HG21	1:123:C:PHE:HE2	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,830)	1:31:C:VAL:HG22	1:123:C:PHE:HE1	9	0.55
(1,830)	1:31:C:VAL:HG22	1:123:C:PHE:HE2	9	0.55
(1,830)	1:31:C:VAL:HG23	1:123:C:PHE:HE1	9	0.55
(1,830)	1:31:C:VAL:HG23	1:123:C:PHE:HE2	9	0.55
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	18	0.55
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	11	0.55
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	9	0.55
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	9	0.55
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	9	0.55
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	9	0.55
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	9	0.55
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	9	0.55
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	9	0.55
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	9	0.55
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	9	0.55
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD21	19	0.55
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD22	19	0.55
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD23	19	0.55
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	13	0.55
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	13	0.55
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	8	0.55
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	8	0.55
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	7	0.55
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	7	0.55
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	7	0.55
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	7	0.55
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	7	0.55
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	7	0.55
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	7	0.55
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	7	0.55
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	7	0.55
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	2	0.55
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	5	0.55
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	13	0.55
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	18	0.54
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	18	0.54
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	18	0.54
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	18	0.54
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	18	0.54
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	18	0.54
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	18	0.54
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	18	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	18	0.54
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	13	0.54
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	5	0.54
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	5	0.54
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	5	0.54
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	5	0.54
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	5	0.54
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	10	0.54
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	10	0.54
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	2	0.54
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	9	0.54
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	19	0.54
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD1	1	0.54
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD2	1	0.54
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD1	1	0.54
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD2	1	0.54
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	20	0.54
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	2	0.54
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	2	0.54
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	2	0.54
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	2	0.54
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	2	0.54
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	2	0.54
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	2	0.54
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	2	0.54
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	2	0.54
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	1	0.54
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	1	0.54
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	1	0.54
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	16	0.54
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	16	0.54
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	16	0.54
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	3	0.54
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	8	0.54
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	9	0.54
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	9	0.54
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	9	0.54
(1,464)	1:32:B:PHE:H	1:34:B:LYS:H	13	0.54
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	17	0.54
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	5	0.54
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	15	0.54
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	20	0.54
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	20	0.54
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	20	0.54
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	20	0.54
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	20	0.54
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	20	0.54
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	20	0.54
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	20	0.54
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	20	0.54
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD21	14	0.54
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD22	14	0.54
(1,105)	1:40:A:VAL:HG11	1:128:A:LEU:HD23	14	0.54
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD21	14	0.54
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD22	14	0.54
(1,105)	1:40:A:VAL:HG12	1:128:A:LEU:HD23	14	0.54
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD21	14	0.54
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD22	14	0.54
(1,105)	1:40:A:VAL:HG13	1:128:A:LEU:HD23	14	0.54
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	5	0.54
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	5	0.54
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD11	5	0.53
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD12	5	0.53
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD13	5	0.53
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD11	5	0.53
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD12	5	0.53
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD13	5	0.53
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD11	5	0.53
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD12	5	0.53
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD13	5	0.53
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	9	0.53
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	9	0.53
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	9	0.53
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	9	0.53
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	9	0.53
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	9	0.53
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	9	0.53
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	9	0.53
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	9	0.53
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	7	0.53
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	15	0.53
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	5	0.53
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	9	0.53
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	9	0.53
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	9	0.53
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	9	0.53
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	19	0.53
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	18	0.53
(1,521)	1:51:B:LEU:H	1:57:B:GLU:H	3	0.53
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	5	0.53
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	5	0.53
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	5	0.53
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	13	0.53
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	8	0.53
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	17	0.53
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	7	0.53
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG21	7	0.53
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG22	7	0.53
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG23	7	0.53
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG21	7	0.53
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG22	7	0.53
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG23	7	0.53
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG21	7	0.53
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG22	7	0.53
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG23	7	0.53
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	20	0.53
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	20	0.53
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	20	0.53
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	18	0.53
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	14	0.53
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	14	0.52
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	14	0.52
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	14	0.52
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	14	0.52
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	14	0.52
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	14	0.52
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	14	0.52
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	14	0.52
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	14	0.52
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	1	0.52
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	1	0.52
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	1	0.52
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	16	0.52
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	16	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	18	0.52
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	18	0.52
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	8	0.52
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	14	0.52
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	14	0.52
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	14	0.52
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	18	0.52
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	6	0.52
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	15	0.52
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	15	0.52
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	10	0.52
(1,640)	1:92:B:THR:H	1:94:B:MET:H	11	0.52
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	5	0.52
(1,478)	1:39:B:GLU:H	1:67:B:SER:H	2	0.52
(1,414)	1:12:B:GLN:H	1:85:B:SER:H	15	0.52
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	7	0.52
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	7	0.52
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	7	0.52
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	7	0.52
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	7	0.52
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	7	0.52
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	20	0.52
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	20	0.52
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	13	0.52
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	4	0.52
(1,182)	1:58:A:VAL:HG11	1:98:A:LEU:HD21	2	0.52
(1,182)	1:58:A:VAL:HG11	1:98:A:LEU:HD22	2	0.52
(1,182)	1:58:A:VAL:HG11	1:98:A:LEU:HD23	2	0.52
(1,182)	1:58:A:VAL:HG12	1:98:A:LEU:HD21	2	0.52
(1,182)	1:58:A:VAL:HG12	1:98:A:LEU:HD22	2	0.52
(1,182)	1:58:A:VAL:HG12	1:98:A:LEU:HD23	2	0.52
(1,182)	1:58:A:VAL:HG13	1:98:A:LEU:HD21	2	0.52
(1,182)	1:58:A:VAL:HG13	1:98:A:LEU:HD22	2	0.52
(1,182)	1:58:A:VAL:HG13	1:98:A:LEU:HD23	2	0.52
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	14	0.52
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	3	0.52
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	3	0.52
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	3	0.52
(1,115)	1:42:A:LEU:HD21	1:43:A:ASP:H	13	0.52
(1,115)	1:42:A:LEU:HD22	1:43:A:ASP:H	13	0.52
(1,115)	1:42:A:LEU:HD23	1:43:A:ASP:H	13	0.52
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	19	0.52
(1,1332)	1:68:D:LEU:HD21	1:73:D:ALA:HB1	15	0.51
(1,1332)	1:68:D:LEU:HD21	1:73:D:ALA:HB2	15	0.51
(1,1332)	1:68:D:LEU:HD21	1:73:D:ALA:HB3	15	0.51
(1,1332)	1:68:D:LEU:HD22	1:73:D:ALA:HB1	15	0.51
(1,1332)	1:68:D:LEU:HD22	1:73:D:ALA:HB2	15	0.51
(1,1332)	1:68:D:LEU:HD22	1:73:D:ALA:HB3	15	0.51
(1,1332)	1:68:D:LEU:HD23	1:73:D:ALA:HB1	15	0.51
(1,1332)	1:68:D:LEU:HD23	1:73:D:ALA:HB2	15	0.51
(1,1332)	1:68:D:LEU:HD23	1:73:D:ALA:HB3	15	0.51
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	15	0.51
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD21	13	0.51
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD22	13	0.51
(1,1279)	1:58:D:VAL:HG11	1:60:D:LEU:HD23	13	0.51
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD21	13	0.51
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD22	13	0.51
(1,1279)	1:58:D:VAL:HG12	1:60:D:LEU:HD23	13	0.51
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD21	13	0.51
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD22	13	0.51
(1,1279)	1:58:D:VAL:HG13	1:60:D:LEU:HD23	13	0.51
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	16	0.51
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	16	0.51
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	16	0.51
(1,1225)	1:42:D:LEU:HD21	1:43:D:ASP:H	2	0.51
(1,1225)	1:42:D:LEU:HD22	1:43:D:ASP:H	2	0.51
(1,1225)	1:42:D:LEU:HD23	1:43:D:ASP:H	2	0.51
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	1	0.51
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	5	0.51
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	19	0.51
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	7	0.51
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	7	0.51
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	7	0.51
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	17	0.51
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	13	0.51
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	13	0.51
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	16	0.51
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	16	0.51
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	14	0.51
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	14	0.51
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	14	0.51
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	14	0.51
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	14	0.51
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	14	0.51
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	14	0.51
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	14	0.51
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	8	0.51
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	15	0.51
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	15	0.51
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	15	0.51
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	15	0.51
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	15	0.51
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	15	0.51
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	15	0.51
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	15	0.51
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	15	0.51
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	4	0.51
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	12	0.51
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	13	0.51
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	5	0.51
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	13	0.51
(1,171)	1:56:A:TYR:H	1:86:A:ILE:H	7	0.51
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD21	8	0.51
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD22	8	0.51
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD23	8	0.51
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD21	8	0.51
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD22	8	0.51
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD23	8	0.51
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD21	8	0.51
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD22	8	0.51
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD23	8	0.51
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	7	0.51
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	7	0.51
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	7	0.51
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	5	0.51
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	15	0.51
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	15	0.51
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	8	0.51
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD1	15	0.5
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD2	15	0.5
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD1	15	0.5
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD2	15	0.5
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD1	15	0.5
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD2	15	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	12	0.5
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	11	0.5
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	19	0.5
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	19	0.5
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	19	0.5
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	8	0.5
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	8	0.5
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	18	0.5
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	11	0.5
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	3	0.5
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG11	12	0.5
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG12	12	0.5
(1,850)	1:40:C:VAL:HG11	1:64:C:VAL:HG13	12	0.5
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG11	12	0.5
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG12	12	0.5
(1,850)	1:40:C:VAL:HG12	1:64:C:VAL:HG13	12	0.5
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG11	12	0.5
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG12	12	0.5
(1,850)	1:40:C:VAL:HG13	1:64:C:VAL:HG13	12	0.5
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	18	0.5
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	20	0.5
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	15	0.5
(1,768)	1:14:C:GLN:H	1:85:C:SER:H	7	0.5
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	10	0.5
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	10	0.5
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	10	0.5
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	5	0.5
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	15	0.5
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	7	0.5
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	7	0.5
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	7	0.5
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	10	0.5
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	19	0.5
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	19	0.5
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	19	0.5
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	19	0.5
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	19	0.5
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	19	0.5
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	19	0.5
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	19	0.5
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	19	0.5
(1,521)	1:51:B:LEU:H	1:57:B:GLU:H	14	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	20	0.5
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	20	0.5
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	20	0.5
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	20	0.5
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	20	0.5
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	20	0.5
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	7	0.5
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	12	0.5
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	12	0.5
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	12	0.5
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	12	0.5
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	12	0.5
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	12	0.5
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	12	0.5
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	12	0.5
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	12	0.5
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	14	0.49
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	14	0.49
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	14	0.49
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD11	4	0.49
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD12	4	0.49
(1,1282)	1:58:D:VAL:HG21	1:98:D:LEU:HD13	4	0.49
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD11	4	0.49
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD12	4	0.49
(1,1282)	1:58:D:VAL:HG22	1:98:D:LEU:HD13	4	0.49
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD11	4	0.49
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD12	4	0.49
(1,1282)	1:58:D:VAL:HG23	1:98:D:LEU:HD13	4	0.49
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	2	0.49
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	2	0.49
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	2	0.49
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	14	0.49
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	14	0.49
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	14	0.49
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	14	0.49
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	14	0.49
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	14	0.49
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD11	14	0.49
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD12	14	0.49
(1,1226)	1:42:D:LEU:HD21	1:44:D:LEU:HD13	14	0.49
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD11	14	0.49
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD12	14	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1226)	1:42:D:LEU:HD22	1:44:D:LEU:HD13	14	0.49
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD11	14	0.49
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD12	14	0.49
(1,1226)	1:42:D:LEU:HD23	1:44:D:LEU:HD13	14	0.49
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	4	0.49
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	4	0.49
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	4	0.49
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	20	0.49
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	1	0.49
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	1	0.49
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	1	0.49
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	1	0.49
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	1	0.49
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	12	0.49
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	12	0.49
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	4	0.49
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	19	0.49
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	11	0.49
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	11	0.49
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	11	0.49
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	11	0.49
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	20	0.49
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	20	0.49
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	20	0.49
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	20	0.49
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	2	0.49
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	6	0.49
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG11	13	0.49
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG12	13	0.49
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG13	13	0.49
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	18	0.49
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	18	0.49
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	18	0.49
(1,830)	1:31:C:VAL:HG21	1:123:C:PHE:HE1	16	0.49
(1,830)	1:31:C:VAL:HG21	1:123:C:PHE:HE2	16	0.49
(1,830)	1:31:C:VAL:HG22	1:123:C:PHE:HE1	16	0.49
(1,830)	1:31:C:VAL:HG22	1:123:C:PHE:HE2	16	0.49
(1,830)	1:31:C:VAL:HG23	1:123:C:PHE:HE1	16	0.49
(1,830)	1:31:C:VAL:HG23	1:123:C:PHE:HE2	16	0.49
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	9	0.49
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	18	0.49
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	18	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	8	0.49
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	16	0.49
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	12	0.49
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	2	0.49
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	2	0.49
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	14	0.49
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	17	0.49
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	20	0.49
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	16	0.49
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	4	0.49
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	4	0.49
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	7	0.49
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	20	0.48
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	13	0.48
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	13	0.48
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	13	0.48
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	13	0.48
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	5	0.48
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	13	0.48
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	13	0.48
(1,931)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	13	0.48
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	13	0.48
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	13	0.48
(1,931)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	13	0.48
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	13	0.48
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	13	0.48
(1,931)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	13	0.48
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	20	0.48
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	5	0.48
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	17	0.48
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	17	0.48
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	17	0.48
(1,826)	1:31:C:VAL:HG11	1:36:C:TRP:HZ3	18	0.48
(1,826)	1:31:C:VAL:HG12	1:36:C:TRP:HZ3	18	0.48
(1,826)	1:31:C:VAL:HG13	1:36:C:TRP:HZ3	18	0.48
(1,824)	1:31:C:VAL:HG11	1:32:C:PHE:H	12	0.48
(1,824)	1:31:C:VAL:HG12	1:32:C:PHE:H	12	0.48
(1,824)	1:31:C:VAL:HG13	1:32:C:PHE:H	12	0.48
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	16	0.48
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	1	0.48
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	1	0.48
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	14	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	3	0.48
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	17	0.48
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	2	0.48
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	2	0.48
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	2	0.48
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	2	0.48
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	2	0.48
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	2	0.48
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	2	0.48
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	2	0.48
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	2	0.48
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	15	0.48
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	6	0.48
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	7	0.48
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	18	0.48
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	12	0.48
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	9	0.48
(1,233)	1:68:A:LEU:HD11	1:73:A:ALA:H	10	0.48
(1,233)	1:68:A:LEU:HD12	1:73:A:ALA:H	10	0.48
(1,233)	1:68:A:LEU:HD13	1:73:A:ALA:H	10	0.48
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	9	0.48
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	11	0.48
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	10	0.48
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	10	0.48
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	10	0.48
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	1	0.48
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	1	0.48
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	4	0.48
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	10	0.48
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD21	16	0.47
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD22	16	0.47
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD23	16	0.47
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD21	16	0.47
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD22	16	0.47
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD23	16	0.47
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD21	16	0.47
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD22	16	0.47
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD23	16	0.47
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	17	0.47
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	20	0.47
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	20	0.47
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	20	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	20	0.47
(1,1234)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	20	0.47
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	20	0.47
(1,1234)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	20	0.47
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	20	0.47
(1,1234)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	20	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	2	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	2	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	2	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	9	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	9	0.47
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	9	0.47
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	8	0.47
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	8	0.47
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	8	0.47
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	7	0.47
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	7	0.47
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	11	0.47
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	11	0.47
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	6	0.47
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	15	0.47
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	15	0.47
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	15	0.47
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	15	0.47
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	15	0.47
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	15	0.47
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	15	0.47
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	15	0.47
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	15	0.47
(1,872)	1:44:C:LEU:HD11	1:63:C:THR:H	19	0.47
(1,872)	1:44:C:LEU:HD12	1:63:C:THR:H	19	0.47
(1,872)	1:44:C:LEU:HD13	1:63:C:THR:H	19	0.47
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	5	0.47
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	5	0.47
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	5	0.47
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	5	0.47
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	5	0.47
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	5	0.47
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	5	0.47
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	5	0.47
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	5	0.47
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	19	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	19	0.47
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	17	0.47
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	17	0.47
(1,706)	1:118:B:VAL:HG11	1:126:B:LEU:H	20	0.47
(1,706)	1:118:B:VAL:HG12	1:126:B:LEU:H	20	0.47
(1,706)	1:118:B:VAL:HG13	1:126:B:LEU:H	20	0.47
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	1	0.47
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	10	0.47
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	9	0.47
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	12	0.47
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	11	0.47
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	11	0.47
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	11	0.47
(1,467)	1:33:B:GLN:H	1:35:B:ASP:H	11	0.47
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	8	0.47
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	5	0.47
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	5	0.47
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	5	0.47
(1,285)	1:92:A:THR:H	1:94:A:MET:H	17	0.47
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG21	18	0.47
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG22	18	0.47
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG23	18	0.47
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG21	18	0.47
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG22	18	0.47
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG23	18	0.47
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG21	18	0.47
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG22	18	0.47
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG23	18	0.47
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	1	0.47
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	1	0.47
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	1	0.47
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	1	0.47
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	18	0.47
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	4	0.46
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	4	0.46
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	4	0.46
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	4	0.46
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	4	0.46
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	4	0.46
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	2	0.46
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	2	0.46
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:91:D:GLY:H	1:95:D:ALA:H	17	0.46
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	16	0.46
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	16	0.46
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	16	0.46
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	9	0.46
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	9	0.46
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	9	0.46
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	9	0.46
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	9	0.46
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	9	0.46
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	9	0.46
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	9	0.46
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	9	0.46
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	2	0.46
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	2	0.46
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	20	0.46
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	20	0.46
(1,1130)	1:140:C:TYR:HD1	1:141:C:LEU:H	13	0.46
(1,1130)	1:140:C:TYR:HD2	1:141:C:LEU:H	13	0.46
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	6	0.46
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	12	0.46
(1,871)	1:44:C:LEU:HD11	1:62:C:VAL:HG21	18	0.46
(1,871)	1:44:C:LEU:HD11	1:62:C:VAL:HG22	18	0.46
(1,871)	1:44:C:LEU:HD11	1:62:C:VAL:HG23	18	0.46
(1,871)	1:44:C:LEU:HD12	1:62:C:VAL:HG21	18	0.46
(1,871)	1:44:C:LEU:HD12	1:62:C:VAL:HG22	18	0.46
(1,871)	1:44:C:LEU:HD12	1:62:C:VAL:HG23	18	0.46
(1,871)	1:44:C:LEU:HD13	1:62:C:VAL:HG21	18	0.46
(1,871)	1:44:C:LEU:HD13	1:62:C:VAL:HG22	18	0.46
(1,871)	1:44:C:LEU:HD13	1:62:C:VAL:HG23	18	0.46
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	12	0.46
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	12	0.46
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	12	0.46
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	19	0.46
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	19	0.46
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	19	0.46
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD21	9	0.46
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD22	9	0.46
(1,652)	1:95:B:ALA:H	1:98:B:LEU:HD23	9	0.46
(1,640)	1:92:B:THR:H	1:94:B:MET:H	9	0.46
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	1	0.46
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	9	0.46
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	5	0.46
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	5	0.46
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	5	0.46
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	5	0.46
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	5	0.46
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	5	0.46
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	5	0.46
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	5	0.46
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	5	0.46
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	8	0.46
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	8	0.46
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	8	0.46
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	8	0.46
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	8	0.46
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	8	0.46
(1,368)	1:128:A:LEU:HD11	1:129:A:ALA:H	20	0.46
(1,368)	1:128:A:LEU:HD12	1:129:A:ALA:H	20	0.46
(1,368)	1:128:A:LEU:HD13	1:129:A:ALA:H	20	0.46
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	15	0.46
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	2	0.46
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	18	0.46
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	5	0.46
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	5	0.46
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	5	0.46
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	10	0.46
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	10	0.46
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	10	0.46
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	1	0.46
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	17	0.46
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	17	0.46
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	6	0.45
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	6	0.45
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	6	0.45
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	6	0.45
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	6	0.45
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	6	0.45
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	14	0.45
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	14	0.45
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	14	0.45
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	6	0.45
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	4	0.45
(1,1014)	1:87:C:ALA:H	1:89:C:ILE:H	10	0.45
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	10	0.45
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	10	0.45
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	10	0.45
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	10	0.45
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	16	0.45
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	20	0.45
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	20	0.45
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	20	0.45
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	13	0.45
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	13	0.45
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	13	0.45
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	12	0.45
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	12	0.45
(1,750)	1:139:B:ASN:H	1:141:B:LEU:H	5	0.45
(1,705)	1:118:B:VAL:HG11	1:119:B:SER:H	17	0.45
(1,705)	1:118:B:VAL:HG12	1:119:B:SER:H	17	0.45
(1,705)	1:118:B:VAL:HG13	1:119:B:SER:H	17	0.45
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	15	0.45
(1,640)	1:92:B:THR:H	1:94:B:MET:H	2	0.45
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	14	0.45
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	19	0.45
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	2	0.45
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	10	0.45
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	11	0.45
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	19	0.45
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	3	0.45
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	3	0.45
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	3	0.45
(1,414)	1:12:B:GLN:H	1:85:B:SER:H	16	0.45
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	11	0.45
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	19	0.45
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	17	0.45
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	16	0.45
(1,120)	1:43:A:ASP:H	1:65:A:THR:H	4	0.45
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	1	0.45
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	1	0.45
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	1	0.45
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	2	0.45
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	4	0.45
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	1	0.45
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	1	0.45
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	15	0.45
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	15	0.45
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	8	0.44
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	8	0.44
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	8	0.44
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD11	6	0.44
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD12	6	0.44
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD13	6	0.44
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD11	6	0.44
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD12	6	0.44
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD13	6	0.44
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	7	0.44
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	7	0.44
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	7	0.44
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	7	0.44
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	7	0.44
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	7	0.44
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	7	0.44
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	7	0.44
(1,1219)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	7	0.44
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	7	0.44
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	7	0.44
(1,1219)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	7	0.44
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	7	0.44
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	7	0.44
(1,1219)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	7	0.44
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	1	0.44
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	1	0.44
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	15	0.44
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	15	0.44
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	2	0.44
(1,1138)	1:10:D:THR:H	1:89:D:ILE:H	20	0.44
(1,1108)	1:131:C:VAL:HG11	1:133:C:PHE:H	3	0.44
(1,1108)	1:131:C:VAL:HG12	1:133:C:PHE:H	3	0.44
(1,1108)	1:131:C:VAL:HG13	1:133:C:PHE:H	3	0.44
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB1	16	0.44
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB2	16	0.44
(1,1105)	1:128:C:LEU:HD11	1:129:C:ALA:HB3	16	0.44
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB1	16	0.44
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB2	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:128:C:LEU:HD12	1:129:C:ALA:HB3	16	0.44
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB1	16	0.44
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB2	16	0.44
(1,1105)	1:128:C:LEU:HD13	1:129:C:ALA:HB3	16	0.44
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	13	0.44
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	13	0.44
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	13	0.44
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	8	0.44
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	7	0.44
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	7	0.44
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	7	0.44
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	7	0.44
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	10	0.44
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	16	0.44
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	1	0.44
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	1	0.44
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	1	0.44
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD21	14	0.44
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD22	14	0.44
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD23	14	0.44
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	2	0.44
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	11	0.44
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	16	0.44
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	16	0.44
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	16	0.44
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG11	8	0.44
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG12	8	0.44
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG13	8	0.44
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	13	0.44
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	15	0.44
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	15	0.44
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	15	0.44
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	15	0.44
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	15	0.44
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	15	0.44
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	15	0.44
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	7	0.44
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	14	0.44
(1,403)	1:9:B:MET:HE1	1:10:B:THR:H	13	0.44
(1,403)	1:9:B:MET:HE2	1:10:B:THR:H	13	0.44
(1,403)	1:9:B:MET:HE3	1:10:B:THR:H	13	0.44
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	10	0.44
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	10	0.44
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	10	0.44
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	10	0.44
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	10	0.44
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	10	0.44
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	13	0.44
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	10	0.44
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	12	0.44
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	1	0.44
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	18	0.44
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	5	0.44
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	5	0.44
(1,1647)	1:128:D:LEU:HD11	2:290:G:TRP:HE3	5	0.43
(1,1647)	1:128:D:LEU:HD12	2:290:G:TRP:HE3	5	0.43
(1,1647)	1:128:D:LEU:HD13	2:290:G:TRP:HE3	5	0.43
(1,1647)	1:128:D:LEU:HD21	2:290:G:TRP:HE3	5	0.43
(1,1647)	1:128:D:LEU:HD22	2:290:G:TRP:HE3	5	0.43
(1,1647)	1:128:D:LEU:HD23	2:290:G:TRP:HE3	5	0.43
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD11	19	0.43
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD12	19	0.43
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD13	19	0.43
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD11	19	0.43
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD12	19	0.43
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD13	19	0.43
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	16	0.43
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	5	0.43
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	16	0.43
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	13	0.43
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	15	0.43
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	14	0.43
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	14	0.43
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	14	0.43
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	3	0.43
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	19	0.43
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	8	0.43
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	8	0.43
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	9	0.43
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	16	0.43
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	6	0.43
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	14	0.43
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	8	0.43
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	8	0.43
(1,630)	1:87:B:ALA:H	1:89:B:ILE:H	3	0.43
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	11	0.43
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	4	0.43
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	17	0.43
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	7	0.43
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	7	0.43
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	18	0.43
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	18	0.43
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	18	0.43
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	18	0.43
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	18	0.43
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	18	0.43
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	7	0.43
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	17	0.43
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	9	0.43
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	2	0.43
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	13	0.43
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	17	0.43
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	16	0.43
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	8	0.42
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	8	0.42
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	8	0.42
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	8	0.42
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	8	0.42
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	8	0.42
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	8	0.42
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	12	0.42
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	10	0.42
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	16	0.42
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	16	0.42
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	16	0.42
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	8	0.42
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	14	0.42
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	14	0.42
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	6	0.42
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	6	0.42
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	17	0.42
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG11	20	0.42
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG12	20	0.42
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG13	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG11	20	0.42
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG12	20	0.42
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG13	20	0.42
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	19	0.42
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	13	0.42
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	11	0.42
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	11	0.42
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	5	0.42
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	5	0.42
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	5	0.42
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	5	0.42
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	5	0.42
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	5	0.42
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	5	0.42
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	5	0.42
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	5	0.42
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	2	0.42
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	17	0.42
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	14	0.42
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	20	0.42
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	19	0.42
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	14	0.42
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	14	0.42
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	14	0.42
(1,384)	1:135:A:ALA:H	1:138:A:MET:H	7	0.42
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	1	0.42
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	8	0.42
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	14	0.42
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	3	0.42
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	10	0.42
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	12	0.42
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	18	0.42
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD11	8	0.42
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD12	8	0.42
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD13	8	0.42
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD11	8	0.42
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD12	8	0.42
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD13	8	0.42
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD11	8	0.42
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD12	8	0.42
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD13	8	0.42
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	19	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	8	0.42
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	9	0.42
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	15	0.42
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	14	0.42
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	20	0.42
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	5	0.41
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	5	0.41
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	5	0.41
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	11	0.41
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	11	0.41
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	11	0.41
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	11	0.41
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	11	0.41
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	11	0.41
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	11	0.41
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	10	0.41
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	17	0.41
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	17	0.41
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	17	0.41
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD1	5	0.41
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD2	5	0.41
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD1	5	0.41
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD2	5	0.41
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG11	6	0.41
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG12	6	0.41
(1,987)	1:74:C:PHE:HE1	1:118:C:VAL:HG13	6	0.41
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG11	6	0.41
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG12	6	0.41
(1,987)	1:74:C:PHE:HE2	1:118:C:VAL:HG13	6	0.41
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	4	0.41
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	2	0.41
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD11	4	0.41
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD12	4	0.41
(1,860)	1:42:C:LEU:HD21	1:44:C:LEU:HD13	4	0.41
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD11	4	0.41
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD12	4	0.41
(1,860)	1:42:C:LEU:HD22	1:44:C:LEU:HD13	4	0.41
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD11	4	0.41
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD12	4	0.41
(1,860)	1:42:C:LEU:HD23	1:44:C:LEU:HD13	4	0.41
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	14	0.41
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	17	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	14	0.41
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	14	0.41
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	14	0.41
(1,719)	1:126:B:LEU:HD21	1:128:B:LEU:H	15	0.41
(1,719)	1:126:B:LEU:HD22	1:128:B:LEU:H	15	0.41
(1,719)	1:126:B:LEU:HD23	1:128:B:LEU:H	15	0.41
(1,716)	1:125:B:GLN:H	1:125:C:GLN:H	5	0.41
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	5	0.41
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	10	0.41
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	12	0.41
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	12	0.41
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	12	0.41
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	12	0.41
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	12	0.41
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	12	0.41
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	12	0.41
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	12	0.41
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	12	0.41
(1,565)	1:60:B:LEU:H	1:82:B:GLY:H	6	0.41
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	19	0.41
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	16	0.41
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	18	0.41
(1,467)	1:33:B:GLN:H	1:35:B:ASP:H	1	0.41
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	11	0.41
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	11	0.41
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	5	0.41
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	2	0.41
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	11	0.41
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	8	0.41
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	5	0.41
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	5	0.41
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	5	0.41
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	5	0.41
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	5	0.41
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	5	0.41
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	5	0.41
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	5	0.41
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	5	0.41
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	6	0.41
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	19	0.41
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	19	0.41
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	2	0.41
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	2	0.41
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	2	0.41
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	13	0.41
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	8	0.41
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	9	0.41
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	12	0.41
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	9	0.41
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	15	0.41
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	16	0.41
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	11	0.4
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	11	0.4
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	11	0.4
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	11	0.4
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	11	0.4
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	11	0.4
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	9	0.4
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	9	0.4
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	9	0.4
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	9	0.4
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	9	0.4
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	9	0.4
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	5	0.4
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	14	0.4
(1,1292)	1:60:D:LEU:HD11	1:62:D:VAL:H	4	0.4
(1,1292)	1:60:D:LEU:HD12	1:62:D:VAL:H	4	0.4
(1,1292)	1:60:D:LEU:HD13	1:62:D:VAL:H	4	0.4
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	3	0.4
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	14	0.4
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	14	0.4
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	3	0.4
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	3	0.4
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	4	0.4
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	4	0.4
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	20	0.4
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	10	0.4
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	10	0.4
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	14	0.4
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	14	0.4
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	3	0.4
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	15	0.4
(1,1050)	1:99:C:GLY:H	1:102:C:CYS:H	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	9	0.4
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	10	0.4
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD21	2	0.4
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD22	2	0.4
(1,925)	1:58:C:VAL:HG11	1:60:C:LEU:HD23	2	0.4
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD21	2	0.4
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD22	2	0.4
(1,925)	1:58:C:VAL:HG12	1:60:C:LEU:HD23	2	0.4
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD21	2	0.4
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD22	2	0.4
(1,925)	1:58:C:VAL:HG13	1:60:C:LEU:HD23	2	0.4
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	1	0.4
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	5	0.4
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	4	0.4
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	10	0.4
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	18	0.4
(1,768)	1:14:C:GLN:H	1:85:C:SER:H	3	0.4
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	2	0.4
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	2	0.4
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	2	0.4
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	2	0.4
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	2	0.4
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	2	0.4
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	2	0.4
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	2	0.4
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	2	0.4
(1,706)	1:118:B:VAL:HG11	1:126:B:LEU:H	17	0.4
(1,706)	1:118:B:VAL:HG12	1:126:B:LEU:H	17	0.4
(1,706)	1:118:B:VAL:HG13	1:126:B:LEU:H	17	0.4
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	8	0.4
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	14	0.4
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	15	0.4
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	17	0.4
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	4	0.4
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	9	0.4
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	8	0.4
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	8	0.4
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	8	0.4
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	8	0.4
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	8	0.4
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	8	0.4
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	8	0.4
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	8	0.4
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	3	0.4
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	5	0.4
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	14	0.4
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	14	0.4
(1,483)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	14	0.4
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	14	0.4
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	14	0.4
(1,483)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	14	0.4
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	14	0.4
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	14	0.4
(1,483)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	14	0.4
(1,446)	1:24:B:GLU:H	1:75:B:LEU:H	10	0.4
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	2	0.4
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	8	0.4
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	17	0.4
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	15	0.4
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	2	0.4
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	10	0.4
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	8	0.4
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	18	0.4
(1,137)	1:47:A:ALA:H	1:60:A:LEU:HD21	9	0.4
(1,137)	1:47:A:ALA:H	1:60:A:LEU:HD22	9	0.4
(1,137)	1:47:A:ALA:H	1:60:A:LEU:HD23	9	0.4
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	3	0.4
(1,111)	1:41:A:LYS:H	1:65:A:THR:H	5	0.4
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	17	0.4
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	17	0.4
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	17	0.4
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	8	0.4
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	16	0.4
(1,3)	1:10:A:THR:H	1:87:A:ALA:H	15	0.4
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD11	10	0.39
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD12	10	0.39
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD13	10	0.39
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD11	10	0.39
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD12	10	0.39
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD13	10	0.39
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD11	10	0.39
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD12	10	0.39
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD13	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	5	0.39
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	5	0.39
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	5	0.39
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	5	0.39
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	5	0.39
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	5	0.39
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	19	0.39
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	19	0.39
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	19	0.39
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	19	0.39
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	19	0.39
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	19	0.39
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	2	0.39
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	2	0.39
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	2	0.39
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	2	0.39
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	2	0.39
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	2	0.39
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	10	0.39
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	7	0.39
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	7	0.39
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	7	0.39
(1,1176)	1:24:D:GLU:H	1:75:D:LEU:H	16	0.39
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	10	0.39
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	10	0.39
(1,1138)	1:10:D:THR:H	1:89:D:ILE:H	4	0.39
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	11	0.39
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	4	0.39
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	20	0.39
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	16	0.39
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	5	0.39
(1,777)	1:17:C:TYR:HE1	1:82:C:GLY:H	1	0.39
(1,777)	1:17:C:TYR:HE2	1:82:C:GLY:H	1	0.39
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	11	0.39
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	20	0.39
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	4	0.39
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	4	0.39
(1,716)	1:125:B:GLN:H	1:125:C:GLN:H	18	0.39
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	8	0.39
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	7	0.39
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	19	0.39
(1,550)	1:58:B:VAL:H	1:84:B:PHE:H	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	7	0.39
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	7	0.39
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	7	0.39
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	7	0.39
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	7	0.39
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	7	0.39
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD11	5	0.39
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD12	5	0.39
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD13	5	0.39
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD11	5	0.39
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD12	5	0.39
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD13	5	0.39
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD11	5	0.39
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD12	5	0.39
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD13	5	0.39
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	11	0.39
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	14	0.39
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	16	0.39
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	5	0.39
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	5	0.39
(1,131)	1:45:A:ASP:H	1:62:A:VAL:H	7	0.39
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	17	0.39
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	1	0.39
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	20	0.39
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	20	0.39
(1,39)	1:20:A:ASP:H	1:79:A:GLN:H	16	0.39
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	5	0.38
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	5	0.38
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	5	0.38
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	16	0.38
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	19	0.38
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	9	0.38
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	13	0.38
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	19	0.38
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	5	0.38
(1,1138)	1:10:D:THR:H	1:89:D:ILE:H	12	0.38
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	13	0.38
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	13	0.38
(1,1022)	1:91:C:GLY:H	1:95:C:ALA:H	16	0.38
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	8	0.38
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	8	0.38
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	8	0.38
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	8	0.38
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	8	0.38
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	8	0.38
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	8	0.38
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	8	0.38
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	13	0.38
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	13	0.38
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	13	0.38
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	13	0.38
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	13	0.38
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	13	0.38
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	13	0.38
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	13	0.38
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	13	0.38
(1,875)	1:45:C:ASP:H	1:61:C:ARG:H	14	0.38
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG11	19	0.38
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG12	19	0.38
(1,861)	1:42:C:LEU:HD21	1:62:C:VAL:HG13	19	0.38
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG11	19	0.38
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG12	19	0.38
(1,861)	1:42:C:LEU:HD22	1:62:C:VAL:HG13	19	0.38
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG11	19	0.38
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG12	19	0.38
(1,861)	1:42:C:LEU:HD23	1:62:C:VAL:HG13	19	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG11	6	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG12	6	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG13	6	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG11	7	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG12	7	0.38
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG13	7	0.38
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	11	0.38
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	12	0.38
(1,777)	1:17:C:TYR:HE1	1:82:C:GLY:H	12	0.38
(1,777)	1:17:C:TYR:HE2	1:82:C:GLY:H	12	0.38
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	5	0.38
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	5	0.38
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	2	0.38
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	13	0.38
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	19	0.38
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	19	0.38
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	19	0.38
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	19	0.38
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	19	0.38
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	19	0.38
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	19	0.38
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	19	0.38
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	3	0.38
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	12	0.38
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	4	0.38
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	1	0.38
(1,475)	1:36:B:TRP:HE3	1:37:B:GLN:H	7	0.38
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	6	0.38
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	6	0.38
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	6	0.38
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	12	0.38
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	12	0.38
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	12	0.38
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	10	0.38
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	16	0.38
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	4	0.38
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	4	0.38
(1,370)	1:128:A:LEU:HD21	1:129:A:ALA:H	11	0.38
(1,370)	1:128:A:LEU:HD22	1:129:A:ALA:H	11	0.38
(1,370)	1:128:A:LEU:HD23	1:129:A:ALA:H	11	0.38
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	19	0.38
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	2	0.38
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	6	0.38
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	6	0.38
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	6	0.38
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	9	0.38
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	15	0.38
(1,120)	1:43:A:ASP:H	1:65:A:THR:H	1	0.38
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	8	0.38
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	20	0.38
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	20	0.38
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	20	0.38
(1,99)	1:39:A:GLU:H	1:67:A:SER:H	16	0.38
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	12	0.38
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	12	0.38
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	12	0.38
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	7	0.38
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	10	0.38
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	6	0.37
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	6	0.37
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	6	0.37
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	6	0.37
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	6	0.37
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	6	0.37
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	6	0.37
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	6	0.37
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	6	0.37
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD11	3	0.37
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD12	3	0.37
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD13	3	0.37
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD21	3	0.37
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD22	3	0.37
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD23	3	0.37
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD11	3	0.37
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD12	3	0.37
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD13	3	0.37
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD21	3	0.37
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD22	3	0.37
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD23	3	0.37
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD11	3	0.37
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD12	3	0.37
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD13	3	0.37
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD21	3	0.37
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD22	3	0.37
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD23	3	0.37
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD11	3	0.37
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD12	3	0.37
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD13	3	0.37
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD21	3	0.37
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD22	3	0.37
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD23	3	0.37
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD11	3	0.37
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD12	3	0.37
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD13	3	0.37
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD21	3	0.37
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD22	3	0.37
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD23	3	0.37
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD11	3	0.37
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD12	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD13	3	0.37
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD21	3	0.37
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD22	3	0.37
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD23	3	0.37
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD11	12	0.37
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD12	12	0.37
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD13	12	0.37
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD21	12	0.37
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD22	12	0.37
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD23	12	0.37
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD11	12	0.37
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD12	12	0.37
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD13	12	0.37
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD21	12	0.37
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD22	12	0.37
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD23	12	0.37
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD11	12	0.37
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD12	12	0.37
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD13	12	0.37
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD21	12	0.37
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD22	12	0.37
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD23	12	0.37
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD11	12	0.37
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD12	12	0.37
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD13	12	0.37
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD21	12	0.37
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD22	12	0.37
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD23	12	0.37
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD11	12	0.37
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD12	12	0.37
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD13	12	0.37
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD21	12	0.37
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD22	12	0.37
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD23	12	0.37
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD11	12	0.37
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD12	12	0.37
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD13	12	0.37
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD21	12	0.37
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD22	12	0.37
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD23	12	0.37
(1,1204)	1:34:D:LYS:H	1:35:D:ASP:H	6	0.37
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	12	0.37
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	12	0.37
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD21	4	0.37
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD22	4	0.37
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD23	4	0.37
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD21	4	0.37
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD22	4	0.37
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD23	4	0.37
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD21	4	0.37
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD22	4	0.37
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD23	4	0.37
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	16	0.37
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	13	0.37
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	3	0.37
(1,875)	1:45:C:ASP:H	1:61:C:ARG:H	7	0.37
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	1	0.37
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	13	0.37
(1,748)	1:138:B:MET:H	1:141:B:LEU:H	17	0.37
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	19	0.37
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	10	0.37
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	18	0.37
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	2	0.37
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	7	0.37
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	16	0.37
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	14	0.37
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD21	3	0.37
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD22	3	0.37
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD23	3	0.37
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	8	0.37
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	3	0.37
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	3	0.37
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	8	0.37
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	8	0.37
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	15	0.37
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	12	0.37
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	12	0.37
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	5	0.37
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	5	0.37
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	5	0.37
(1,77)	1:31:A:VAL:HG11	1:36:A:TRP:HZ3	7	0.37
(1,77)	1:31:A:VAL:HG12	1:36:A:TRP:HZ3	7	0.37
(1,77)	1:31:A:VAL:HG13	1:36:A:TRP:HZ3	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	3	0.37
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	5	0.37
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	19	0.37
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	19	0.37
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	20	0.37
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	1	0.36
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	2	0.36
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	2	0.36
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	2	0.36
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	2	0.36
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	2	0.36
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	2	0.36
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	5	0.36
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	5	0.36
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	5	0.36
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	5	0.36
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	5	0.36
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	5	0.36
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE1	1	0.36
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE2	1	0.36
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE1	1	0.36
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE2	1	0.36
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD11	10	0.36
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD12	10	0.36
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD13	10	0.36
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD21	10	0.36
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD22	10	0.36
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD23	10	0.36
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD11	10	0.36
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD12	10	0.36
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD13	10	0.36
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD21	10	0.36
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD22	10	0.36
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD23	10	0.36
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD11	10	0.36
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD12	10	0.36
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD13	10	0.36
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD21	10	0.36
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD22	10	0.36
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD23	10	0.36
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	7	0.36
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	17	0.36
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	17	0.36
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	9	0.36
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	9	0.36
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	20	0.36
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	8	0.36
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	8	0.36
(1,1130)	1:140:C:TYR:HD1	1:141:C:LEU:H	3	0.36
(1,1130)	1:140:C:TYR:HD2	1:141:C:LEU:H	3	0.36
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	5	0.36
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	19	0.36
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	18	0.36
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	17	0.36
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	17	0.36
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	17	0.36
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD1	13	0.36
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD2	13	0.36
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD1	13	0.36
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD2	13	0.36
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD1	13	0.36
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD2	13	0.36
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	4	0.36
(1,644)	1:93:B:GLN:H	1:96:B:HIS:H	9	0.36
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	14	0.36
(1,550)	1:58:B:VAL:H	1:84:B:PHE:H	6	0.36
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	17	0.36
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	18	0.36
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	9	0.36
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	5	0.36
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	18	0.36
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	6	0.36
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	15	0.36
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	3	0.36
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	13	0.36
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	11	0.36
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	6	0.36
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	8	0.36
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	13	0.36
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	13	0.36
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	13	0.36
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	13	0.36
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	13	0.36
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	13	0.36
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	13	0.36
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	13	0.36
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	14	0.36
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	18	0.36
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	3	0.36
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	20	0.36
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	16	0.36
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	16	0.36
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	2	0.36
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	15	0.36
(1,19)	1:14:A:GLN:H	1:85:A:SER:H	8	0.36
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	15	0.36
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD1	16	0.35
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD2	16	0.35
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD1	16	0.35
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD2	16	0.35
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD1	16	0.35
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD2	16	0.35
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD21	13	0.35
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD22	13	0.35
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD23	13	0.35
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD21	13	0.35
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD22	13	0.35
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD23	13	0.35
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD21	13	0.35
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD22	13	0.35
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD23	13	0.35
(1,1473)	1:134:D:ASP:H	1:136:D:LEU:H	20	0.35
(1,1412)	1:99:D:GLY:H	1:102:D:CYS:H	1	0.35
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	18	0.35
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	18	0.35
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	18	0.35
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	18	0.35
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	18	0.35
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	18	0.35
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	18	0.35
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	18	0.35
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	18	0.35
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	5	0.35
(1,1248)	1:49:D:SER:H	1:59:D:VAL:H	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	18	0.35
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	18	0.35
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	18	0.35
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	18	0.35
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	18	0.35
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	18	0.35
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	18	0.35
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	18	0.35
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	18	0.35
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	17	0.35
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	17	0.35
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	17	0.35
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	19	0.35
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	19	0.35
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	5	0.35
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	5	0.35
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD21	16	0.35
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD22	16	0.35
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD23	16	0.35
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD21	16	0.35
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD22	16	0.35
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD23	16	0.35
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD21	16	0.35
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD22	16	0.35
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD23	16	0.35
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	12	0.35
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	13	0.35
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	4	0.35
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	13	0.35
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD11	13	0.35
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD12	13	0.35
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD13	13	0.35
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD11	13	0.35
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD12	13	0.35
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD13	13	0.35
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD11	13	0.35
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD12	13	0.35
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD13	13	0.35
(1,843)	1:39:C:GLU:H	1:40:C:VAL:H	11	0.35
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	3	0.35
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	9	0.35
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	11	0.35
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	11	0.35
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	11	0.35
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	12	0.35
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	12	0.35
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	12	0.35
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	7	0.35
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	15	0.35
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	6	0.35
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	16	0.35
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	11	0.35
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	13	0.35
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	12	0.35
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	2	0.35
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	20	0.35
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	6	0.35
(1,506)	1:45:B:ASP:H	1:63:B:THR:H	14	0.35
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	18	0.35
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	15	0.35
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	18	0.35
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	10	0.35
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	13	0.35
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	13	0.35
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	13	0.35
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	13	0.35
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	13	0.35
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	13	0.35
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	3	0.35
(1,357)	1:121:A:GLY:H	1:123:A:PHE:H	14	0.35
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	5	0.35
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	19	0.35
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	6	0.35
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	15	0.35
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	5	0.35
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	11	0.35
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	9	0.35
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	7	0.35
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	20	0.35
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	18	0.35
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	18	0.35
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	18	0.35
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	18	0.35
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	14	0.35
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	15	0.35
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	19	0.35
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	2	0.35
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	3	0.35
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	8	0.35
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	10	0.35
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	11	0.35
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	9	0.35
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	9	0.35
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	20	0.34
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	20	0.34
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	20	0.34
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	20	0.34
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	20	0.34
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	20	0.34
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	20	0.34
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	20	0.34
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	20	0.34
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD11	19	0.34
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD12	19	0.34
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD13	19	0.34
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD11	19	0.34
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD12	19	0.34
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD13	19	0.34
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD11	19	0.34
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD12	19	0.34
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD13	19	0.34
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD11	13	0.34
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD12	13	0.34
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD13	13	0.34
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD11	13	0.34
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD12	13	0.34
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD13	13	0.34
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD11	13	0.34
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD12	13	0.34
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD13	13	0.34
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	1	0.34
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	1	0.34
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	1	0.34
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	20	0.34
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	20	0.34
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	19	0.34
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	7	0.34
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	14	0.34
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	15	0.34
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	15	0.34
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	11	0.34
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	4	0.34
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	4	0.34
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	8	0.34
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	8	0.34
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	17	0.34
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	17	0.34
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	17	0.34
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	14	0.34
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	19	0.34
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB1	16	0.34
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB2	16	0.34
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB3	16	0.34
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD21	12	0.34
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD22	12	0.34
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD23	12	0.34
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD11	3	0.34
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD12	3	0.34
(1,838)	1:35:C:ASP:H	1:68:C:LEU:HD13	3	0.34
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	10	0.34
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	19	0.34
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	15	0.34
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	16	0.34
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	15	0.34
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	15	0.34
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	10	0.34
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	10	0.34
(1,716)	1:125:B:GLN:H	1:125:C:GLN:H	15	0.34
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	4	0.34
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	2	0.34
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	2	0.34
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	2	0.34
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	2	0.34
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	2	0.34
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	2	0.34
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	2	0.34
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	2	0.34
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	2	0.34
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	19	0.34
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	7	0.34
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	17	0.34
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	5	0.34
(1,536)	1:55:B:VAL:H	1:56:B:TYR:H	13	0.34
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	16	0.34
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD11	9	0.34
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD12	9	0.34
(1,473)	1:36:B:TRP:H	1:68:B:LEU:HD13	9	0.34
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	17	0.34
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	4	0.34
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	4	0.34
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	9	0.34
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	19	0.34
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	20	0.34
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	3	0.34
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	10	0.34
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	5	0.34
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	5	0.34
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	17	0.34
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	6	0.34
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	11	0.34
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	9	0.34
(1,99)	1:39:A:GLU:H	1:67:A:SER:H	3	0.34
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	18	0.34
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	5	0.34
(1,19)	1:14:A:GLN:H	1:85:A:SER:H	19	0.34
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	1	0.33
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	1	0.33
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	1	0.33
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	1	0.33
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	1	0.33
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	1	0.33
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	19	0.33
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	19	0.33
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	19	0.33
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	19	0.33
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	19	0.33
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD11	6	0.33
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD12	6	0.33
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD13	6	0.33
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	11	0.33
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	11	0.33
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	11	0.33
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	11	0.33
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	11	0.33
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	11	0.33
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	14	0.33
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	14	0.33
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	14	0.33
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	18	0.33
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	20	0.33
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD21	5	0.33
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD22	5	0.33
(1,1280)	1:58:D:VAL:HG11	1:98:D:LEU:HD23	5	0.33
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD21	5	0.33
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD22	5	0.33
(1,1280)	1:58:D:VAL:HG12	1:98:D:LEU:HD23	5	0.33
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD21	5	0.33
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD22	5	0.33
(1,1280)	1:58:D:VAL:HG13	1:98:D:LEU:HD23	5	0.33
(1,1191)	1:31:D:VAL:HG11	1:35:D:ASP:H	6	0.33
(1,1191)	1:31:D:VAL:HG12	1:35:D:ASP:H	6	0.33
(1,1191)	1:31:D:VAL:HG13	1:35:D:ASP:H	6	0.33
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	18	0.33
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	7	0.33
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	14	0.33
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	14	0.33
(1,1019)	1:90:C:GLU:H	1:94:C:MET:H	14	0.33
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	4	0.33
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	5	0.33
(1,825)	1:31:C:VAL:HG11	1:32:C:PHE:HD1	18	0.33
(1,825)	1:31:C:VAL:HG11	1:32:C:PHE:HD2	18	0.33
(1,825)	1:31:C:VAL:HG12	1:32:C:PHE:HD1	18	0.33
(1,825)	1:31:C:VAL:HG12	1:32:C:PHE:HD2	18	0.33
(1,825)	1:31:C:VAL:HG13	1:32:C:PHE:HD1	18	0.33
(1,825)	1:31:C:VAL:HG13	1:32:C:PHE:HD2	18	0.33
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	9	0.33
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	18	0.33
(1,732)	1:134:B:ASP:H	1:136:B:LEU:H	6	0.33
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	7	0.33
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	7	0.33
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	7	0.33
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	7	0.33
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	7	0.33
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	7	0.33
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	7	0.33
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	7	0.33
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	7	0.33
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	20	0.33
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	13	0.33
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	9	0.33
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	8	0.33
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	20	0.33
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	12	0.33
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	17	0.33
(1,496)	1:43:B:ASP:H	1:65:B:THR:H	8	0.33
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	3	0.33
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	20	0.33
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	20	0.33
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	4	0.33
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	7	0.33
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	15	0.33
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	10	0.33
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	13	0.33
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	16	0.33
(1,111)	1:41:A:LYS:H	1:65:A:THR:H	13	0.33
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	16	0.33
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	16	0.33
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	16	0.33
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	16	0.33
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	16	0.33
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	1	0.33
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	10	0.32
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	10	0.32
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	10	0.32
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	2	0.32
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	2	0.32
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	2	0.32
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	2	0.32
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	2	0.32
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	2	0.32
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	2	0.32
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	2	0.32
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD11	2	0.32
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD12	2	0.32
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD13	2	0.32
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD21	2	0.32
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD22	2	0.32
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD23	2	0.32
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD11	2	0.32
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD12	2	0.32
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD13	2	0.32
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD21	2	0.32
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD22	2	0.32
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD23	2	0.32
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD11	2	0.32
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD12	2	0.32
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD13	2	0.32
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD21	2	0.32
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD22	2	0.32
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD23	2	0.32
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD11	2	0.32
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD12	2	0.32
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD13	2	0.32
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD21	2	0.32
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD22	2	0.32
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD23	2	0.32
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD11	2	0.32
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD12	2	0.32
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD13	2	0.32
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD21	2	0.32
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD22	2	0.32
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD23	2	0.32
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD11	2	0.32
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD12	2	0.32
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD13	2	0.32
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD21	2	0.32
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD22	2	0.32
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD23	2	0.32
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	3	0.32
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	3	0.32
(1,1474)	1:134:D:ASP:H	1:137:D:PHE:H	15	0.32
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	13	0.32
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	9	0.32
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	12	0.32
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	10	0.32
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	10	0.32
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	10	0.32
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	10	0.32
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	10	0.32
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	10	0.32
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	10	0.32
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	10	0.32
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	10	0.32
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	17	0.32
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	18	0.32
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	1	0.32
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	12	0.32
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	12	0.32
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	12	0.32
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	7	0.32
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	7	0.32
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	7	0.32
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	7	0.32
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	7	0.32
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	7	0.32
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	7	0.32
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	7	0.32
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	7	0.32
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	16	0.32
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	11	0.32
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	11	0.32
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	11	0.32
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	8	0.32
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	8	0.32
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	8	0.32
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	8	0.32
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	8	0.32
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	8	0.32
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	9	0.32
(1,1109)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	9	0.32
(1,1109)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	9	0.32
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	9	0.32
(1,1109)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	9	0.32
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	4	0.32
(1,1022)	1:91:C:GLY:H	1:95:C:ALA:H	2	0.32
(1,1019)	1:90:C:GLU:H	1:94:C:MET:H	5	0.32
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	18	0.32
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	5	0.32
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	2	0.32
(1,875)	1:45:C:ASP:H	1:61:C:ARG:H	8	0.32
(1,859)	1:42:C:LEU:HD21	1:43:C:ASP:H	8	0.32
(1,859)	1:42:C:LEU:HD22	1:43:C:ASP:H	8	0.32
(1,859)	1:42:C:LEU:HD23	1:43:C:ASP:H	8	0.32
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	13	0.32
(1,843)	1:39:C:GLU:H	1:40:C:VAL:H	3	0.32
(1,843)	1:39:C:GLU:H	1:40:C:VAL:H	12	0.32
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD21	20	0.32
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD22	20	0.32
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD23	20	0.32
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	17	0.32
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	4	0.32
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	7	0.32
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	14	0.32
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	9	0.32
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	9	0.32
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	9	0.32
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	17	0.32
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	17	0.32
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	17	0.32
(1,768)	1:14:C:GLN:H	1:85:C:SER:H	11	0.32
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	1	0.32
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	1	0.32
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	16	0.32
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	16	0.32
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG21	7	0.32
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG22	7	0.32
(1,724)	1:128:B:LEU:HD21	1:131:B:VAL:HG23	7	0.32
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG21	7	0.32
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG22	7	0.32
(1,724)	1:128:B:LEU:HD22	1:131:B:VAL:HG23	7	0.32
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG21	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG22	7	0.32
(1,724)	1:128:B:LEU:HD23	1:131:B:VAL:HG23	7	0.32
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	3	0.32
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	20	0.32
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	16	0.32
(1,641)	1:92:B:THR:H	1:95:B:ALA:H	2	0.32
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	9	0.32
(1,550)	1:58:B:VAL:H	1:84:B:PHE:H	16	0.32
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	10	0.32
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	4	0.32
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	9	0.32
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	14	0.32
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	5	0.32
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	5	0.32
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD21	4	0.32
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD22	4	0.32
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD23	4	0.32
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD21	4	0.32
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD22	4	0.32
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD23	4	0.32
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD21	4	0.32
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD22	4	0.32
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD23	4	0.32
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	4	0.32
(1,357)	1:121:A:GLY:H	1:123:A:PHE:H	13	0.32
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	16	0.32
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	1	0.32
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	4	0.32
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	7	0.32
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	12	0.32
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	2	0.32
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	18	0.32
(1,302)	1:96:A:HIS:H	1:99:A:GLY:H	6	0.32
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE1	10	0.32
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE2	10	0.32
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE3	10	0.32
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	9	0.32
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	19	0.32
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	14	0.32
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	19	0.32
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	3	0.32
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:51:A:LEU:H	1:55:A:VAL:H	10	0.32
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	17	0.32
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	13	0.32
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	5	0.32
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	13	0.32
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	20	0.32
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	1	0.32
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	17	0.32
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	20	0.32
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG21	6	0.31
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG22	6	0.31
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG23	6	0.31
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG21	6	0.31
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG22	6	0.31
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG23	6	0.31
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG21	6	0.31
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG22	6	0.31
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG23	6	0.31
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	20	0.31
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	20	0.31
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	20	0.31
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	20	0.31
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	20	0.31
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	20	0.31
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG21	17	0.31
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG22	17	0.31
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG23	17	0.31
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG21	17	0.31
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG22	17	0.31
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG23	17	0.31
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG21	17	0.31
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG22	17	0.31
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG23	17	0.31
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	14	0.31
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	1	0.31
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	2	0.31
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	8	0.31
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	3	0.31
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	3	0.31
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	10	0.31
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	15	0.31
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	20	0.31
(1,1037)	1:96:C:HIS:H	1:99:C:GLY:H	15	0.31
(1,1022)	1:91:C:GLY:H	1:95:C:ALA:H	4	0.31
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	18	0.31
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	12	0.31
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD11	2	0.31
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD12	2	0.31
(1,856)	1:42:C:LEU:HD11	1:44:C:LEU:HD13	2	0.31
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD11	2	0.31
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD12	2	0.31
(1,856)	1:42:C:LEU:HD12	1:44:C:LEU:HD13	2	0.31
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD11	2	0.31
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD12	2	0.31
(1,856)	1:42:C:LEU:HD13	1:44:C:LEU:HD13	2	0.31
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	12	0.31
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	12	0.31
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	12	0.31
(1,843)	1:39:C:GLU:H	1:40:C:VAL:H	13	0.31
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	5	0.31
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	5	0.31
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	5	0.31
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	17	0.31
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	8	0.31
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	8	0.31
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	8	0.31
(1,716)	1:125:B:GLN:H	1:125:C:GLN:H	2	0.31
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	4	0.31
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	13	0.31
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	16	0.31
(1,496)	1:43:B:ASP:H	1:65:B:THR:H	1	0.31
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	5	0.31
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	5	0.31
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	5	0.31
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	3	0.31
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	4	0.31
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	19	0.31
(1,381)	1:134:A:ASP:H	1:136:A:LEU:H	14	0.31
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	8	0.31
(1,368)	1:128:A:LEU:HD11	1:129:A:ALA:H	1	0.31
(1,368)	1:128:A:LEU:HD12	1:129:A:ALA:H	1	0.31
(1,368)	1:128:A:LEU:HD13	1:129:A:ALA:H	1	0.31
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	9	0.31
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	11	0.31
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	6	0.31
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	13	0.31
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	13	0.31
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	15	0.31
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	12	0.31
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE1	6	0.31
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE2	6	0.31
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	11	0.31
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	18	0.31
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG11	12	0.31
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG12	12	0.31
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG13	12	0.31
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	1	0.31
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	1	0.31
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	1	0.31
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	1	0.31
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	1	0.31
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	1	0.31
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	1	0.31
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	1	0.31
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	1	0.31
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	6	0.31
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	8	0.31
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	8	0.31
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	8	0.31
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	5	0.31
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	14	0.31
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	10	0.31
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	13	0.31
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	13	0.31
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	15	0.31
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD11	9	0.3
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD12	9	0.3
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD13	9	0.3
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	7	0.3
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	7	0.3
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	7	0.3
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	7	0.3
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	7	0.3
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1653)	1:13:C:ILE:HD11	2:306:G:VAL:HG21	20	0.3
(1,1653)	1:13:C:ILE:HD11	2:306:G:VAL:HG22	20	0.3
(1,1653)	1:13:C:ILE:HD11	2:306:G:VAL:HG23	20	0.3
(1,1653)	1:13:C:ILE:HD12	2:306:G:VAL:HG21	20	0.3
(1,1653)	1:13:C:ILE:HD12	2:306:G:VAL:HG22	20	0.3
(1,1653)	1:13:C:ILE:HD12	2:306:G:VAL:HG23	20	0.3
(1,1653)	1:13:C:ILE:HD13	2:306:G:VAL:HG21	20	0.3
(1,1653)	1:13:C:ILE:HD13	2:306:G:VAL:HG22	20	0.3
(1,1653)	1:13:C:ILE:HD13	2:306:G:VAL:HG23	20	0.3
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	17	0.3
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	17	0.3
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	17	0.3
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD21	1	0.3
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD22	1	0.3
(1,1517)	1:94:A:MET:HE1	2:277:E:LEU:HD23	1	0.3
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD21	1	0.3
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD22	1	0.3
(1,1517)	1:94:A:MET:HE2	2:277:E:LEU:HD23	1	0.3
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD21	1	0.3
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD22	1	0.3
(1,1517)	1:94:A:MET:HE3	2:277:E:LEU:HD23	1	0.3
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	9	0.3
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	7	0.3
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	7	0.3
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	7	0.3
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	5	0.3
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	5	0.3
(1,1283)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	5	0.3
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	5	0.3
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	5	0.3
(1,1283)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	5	0.3
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	5	0.3
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	5	0.3
(1,1283)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	5	0.3
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	12	0.3
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	3	0.3
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	3	0.3
(1,1197)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	3	0.3
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	3	0.3
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	3	0.3
(1,1197)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	3	0.3
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	3	0.3
(1,1197)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	3	0.3
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	4	0.3
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	4	0.3
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	6	0.3
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	6	0.3
(1,1170)	1:23:D:PHE:HD1	1:24:D:GLU:H	17	0.3
(1,1170)	1:23:D:PHE:HD2	1:24:D:GLU:H	17	0.3
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	13	0.3
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	13	0.3
(1,1130)	1:140:C:TYR:HD1	1:141:C:LEU:H	10	0.3
(1,1130)	1:140:C:TYR:HD2	1:141:C:LEU:H	10	0.3
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	8	0.3
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	8	0.3
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	8	0.3
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	6	0.3
(1,1033)	1:95:C:ALA:H	1:98:C:LEU:H	7	0.3
(1,1028)	1:93:C:GLN:H	1:96:C:HIS:H	2	0.3
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	3	0.3
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	12	0.3
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	8	0.3
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	15	0.3
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	19	0.3
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	12	0.3
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	8	0.3
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	14	0.3
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	11	0.3
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	11	0.3
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	11	0.3
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	11	0.3
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	11	0.3
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	11	0.3
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	11	0.3
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	11	0.3
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	11	0.3
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD21	19	0.3
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD22	19	0.3
(1,864)	1:42:C:LEU:HD21	1:128:C:LEU:HD23	19	0.3
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD21	19	0.3
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD22	19	0.3
(1,864)	1:42:C:LEU:HD22	1:128:C:LEU:HD23	19	0.3
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD21	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD22	19	0.3
(1,864)	1:42:C:LEU:HD23	1:128:C:LEU:HD23	19	0.3
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	8	0.3
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	1	0.3
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	14	0.3
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	14	0.3
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	14	0.3
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	15	0.3
(1,660)	1:97:B:CYS:H	1:101:B:TYR:H	8	0.3
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	4	0.3
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	11	0.3
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	20	0.3
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	18	0.3
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	12	0.3
(1,521)	1:51:B:LEU:H	1:57:B:GLU:H	8	0.3
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	6	0.3
(1,496)	1:43:B:ASP:H	1:65:B:THR:H	16	0.3
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD21	11	0.3
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD22	11	0.3
(1,494)	1:43:B:ASP:H	1:44:B:LEU:HD23	11	0.3
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	4	0.3
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	19	0.3
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	11	0.3
(1,384)	1:135:A:ALA:H	1:138:A:MET:H	17	0.3
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	10	0.3
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	15	0.3
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	3	0.3
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	4	0.3
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	14	0.3
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	4	0.3
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	14	0.3
(1,124)	1:44:A:LEU:HD11	1:46:A:THR:H	17	0.3
(1,124)	1:44:A:LEU:HD12	1:46:A:THR:H	17	0.3
(1,124)	1:44:A:LEU:HD13	1:46:A:THR:H	17	0.3
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	9	0.3
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	9	0.3
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	9	0.3
(1,120)	1:43:A:ASP:H	1:65:A:THR:H	2	0.3
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	15	0.3
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	17	0.3
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	17	0.3
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	2	0.3
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	2	0.3
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	2	0.3
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	15	0.3
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	15	0.3
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	15	0.3
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	19	0.3
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	19	0.3
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	19	0.3
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	17	0.3
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	12	0.3
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	12	0.3
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	8	0.3
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	15	0.29
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	15	0.29
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	15	0.29
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	11	0.29
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	11	0.29
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	11	0.29
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	11	0.29
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	11	0.29
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	11	0.29
(1,1666)	1:129:B:ALA:HB1	2:290:H:TRP:HZ3	8	0.29
(1,1666)	1:129:B:ALA:HB2	2:290:H:TRP:HZ3	8	0.29
(1,1666)	1:129:B:ALA:HB3	2:290:H:TRP:HZ3	8	0.29
(1,1637)	1:98:D:LEU:HD11	2:281:G:PHE:HZ	4	0.29
(1,1637)	1:98:D:LEU:HD12	2:281:G:PHE:HZ	4	0.29
(1,1637)	1:98:D:LEU:HD13	2:281:G:PHE:HZ	4	0.29
(1,1637)	1:98:D:LEU:HD21	2:281:G:PHE:HZ	4	0.29
(1,1637)	1:98:D:LEU:HD22	2:281:G:PHE:HZ	4	0.29
(1,1637)	1:98:D:LEU:HD23	2:281:G:PHE:HZ	4	0.29
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD11	8	0.29
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD12	8	0.29
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD13	8	0.29
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD21	8	0.29
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD22	8	0.29
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD23	8	0.29
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD11	8	0.29
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD12	8	0.29
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD13	8	0.29
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD21	8	0.29
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD22	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD23	8	0.29
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD11	8	0.29
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD12	8	0.29
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD13	8	0.29
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD21	8	0.29
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD22	8	0.29
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD23	8	0.29
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD11	8	0.29
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD12	8	0.29
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD13	8	0.29
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD21	8	0.29
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD22	8	0.29
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD23	8	0.29
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD11	8	0.29
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD12	8	0.29
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD13	8	0.29
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD21	8	0.29
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD22	8	0.29
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD23	8	0.29
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD11	8	0.29
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD12	8	0.29
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD13	8	0.29
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD21	8	0.29
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD22	8	0.29
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD23	8	0.29
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	17	0.29
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	17	0.29
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	17	0.29
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	17	0.29
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	17	0.29
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	17	0.29
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD1	12	0.29
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD2	12	0.29
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD1	12	0.29
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD2	12	0.29
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD1	12	0.29
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD2	12	0.29
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	1	0.29
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	1	0.29
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	1	0.29
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	1	0.29
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	1	0.29
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	12	0.29
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	12	0.29
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	12	0.29
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	12	0.29
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	12	0.29
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	12	0.29
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	18	0.29
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	18	0.29
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	18	0.29
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	18	0.29
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	3	0.29
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	3	0.29
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	3	0.29
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	3	0.29
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	3	0.29
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	3	0.29
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	3	0.29
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	1	0.29
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	1	0.29
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	1	0.29
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	1	0.29
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	1	0.29
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	1	0.29
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	1	0.29
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	1	0.29
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	1	0.29
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	13	0.29
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	14	0.29
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	5	0.29
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	1	0.29
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	1	0.29
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	1	0.29
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	1	0.29
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	1	0.29
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	1	0.29
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	1	0.29
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	1	0.29
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	1	0.29
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	9	0.29
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	9	0.29
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	12	0.29
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	12	0.29
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	7	0.29
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	12	0.29
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	9	0.29
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	9	0.29
(1,1138)	1:10:D:THR:H	1:89:D:ILE:H	7	0.29
(1,1136)	1:10:D:THR:H	1:87:D:ALA:H	2	0.29
(1,1088)	1:118:C:VAL:HG21	1:126:C:LEU:H	12	0.29
(1,1088)	1:118:C:VAL:HG22	1:126:C:LEU:H	12	0.29
(1,1088)	1:118:C:VAL:HG23	1:126:C:LEU:H	12	0.29
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	17	0.29
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	10	0.29
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	20	0.29
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	10	0.29
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	12	0.29
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	12	0.29
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	12	0.29
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	17	0.29
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	17	0.29
(1,744)	1:137:B:PHE:H	1:140:B:TYR:H	3	0.29
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD1	4	0.29
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD2	4	0.29
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD1	4	0.29
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD2	4	0.29
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD1	4	0.29
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD2	4	0.29
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD1	18	0.29
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD2	18	0.29
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD1	18	0.29
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD2	18	0.29
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD1	18	0.29
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD2	18	0.29
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	16	0.29
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	11	0.29
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	13	0.29
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	11	0.29
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	11	0.29
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	7	0.29
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	7	0.29
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	7	0.29
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	7	0.29
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	7	0.29
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	7	0.29
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	7	0.29
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	7	0.29
(1,550)	1:58:B:VAL:H	1:84:B:PHE:H	5	0.29
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	5	0.29
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	2	0.29
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	2	0.29
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	14	0.29
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	17	0.29
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	6	0.29
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	4	0.29
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	3	0.29
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	5	0.29
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	15	0.29
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	15	0.29
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	20	0.29
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	9	0.29
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	9	0.29
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	9	0.29
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	19	0.29
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	9	0.29
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG21	10	0.29
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG22	10	0.29
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG23	10	0.29
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	13	0.29
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG11	1	0.29
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG12	1	0.29
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG13	1	0.29
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	5	0.29
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	17	0.29
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	12	0.29
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	12	0.29
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	12	0.29
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE1	14	0.29
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE2	14	0.29
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE1	14	0.29
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE2	14	0.29
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE1	14	0.29
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE2	14	0.29
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	7	0.29
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	11	0.29
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	16	0.29
(1,50)	1:23:A:PHE:H	1:21:B:ILE:H	20	0.29
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	18	0.29
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	2	0.29
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	18	0.28
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	18	0.28
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	18	0.28
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	18	0.28
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	18	0.28
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	18	0.28
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD11	8	0.28
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD12	8	0.28
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD13	8	0.28
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD21	8	0.28
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD22	8	0.28
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD23	8	0.28
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD11	8	0.28
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD12	8	0.28
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD13	8	0.28
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD21	8	0.28
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD22	8	0.28
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD23	8	0.28
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD11	8	0.28
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD12	8	0.28
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD13	8	0.28
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD21	8	0.28
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD22	8	0.28
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD23	8	0.28
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	13	0.28
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	13	0.28
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	13	0.28
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	13	0.28
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	13	0.28
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	13	0.28
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	8	0.28
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	8	0.28
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	8	0.28
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	8	0.28
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	8	0.28
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	8	0.28
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	8	0.28
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	8	0.28
(1,1462)	1:128:D:LEU:HD11	1:129:D:ALA:H	6	0.28
(1,1462)	1:128:D:LEU:HD12	1:129:D:ALA:H	6	0.28
(1,1462)	1:128:D:LEU:HD13	1:129:D:ALA:H	6	0.28
(1,1382)	1:91:D:GLY:H	1:95:D:ALA:H	7	0.28
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	20	0.28
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	20	0.28
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	20	0.28
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	20	0.28
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD21	6	0.28
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD22	6	0.28
(1,1100)	1:126:C:LEU:HD11	1:128:C:LEU:HD23	6	0.28
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD21	6	0.28
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD22	6	0.28
(1,1100)	1:126:C:LEU:HD12	1:128:C:LEU:HD23	6	0.28
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD21	6	0.28
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD22	6	0.28
(1,1100)	1:126:C:LEU:HD13	1:128:C:LEU:HD23	6	0.28
(1,1099)	1:126:C:LEU:HD11	1:128:C:LEU:H	2	0.28
(1,1099)	1:126:C:LEU:HD12	1:128:C:LEU:H	2	0.28
(1,1099)	1:126:C:LEU:HD13	1:128:C:LEU:H	2	0.28
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	9	0.28
(1,1042)	1:98:C:LEU:H	1:99:C:GLY:H	15	0.28
(1,1042)	1:98:C:LEU:H	1:99:C:GLY:H	20	0.28
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	4	0.28
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	7	0.28
(1,986)	1:74:C:PHE:HD1	1:123:C:PHE:HE1	6	0.28
(1,986)	1:74:C:PHE:HD1	1:123:C:PHE:HE2	6	0.28
(1,986)	1:74:C:PHE:HD2	1:123:C:PHE:HE1	6	0.28
(1,986)	1:74:C:PHE:HD2	1:123:C:PHE:HE2	6	0.28
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	7	0.28
(1,876)	1:45:C:ASP:H	1:63:C:THR:H	12	0.28
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG11	1	0.28
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG12	1	0.28
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG13	1	0.28
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	9	0.28
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	9	0.28
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	9	0.28
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	11	0.28
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	11	0.28
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	2	0.28
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	14	0.28
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	5	0.28
(1,739)	1:136:B:LEU:HD21	1:137:B:PHE:H	4	0.28
(1,739)	1:136:B:LEU:HD22	1:137:B:PHE:H	4	0.28
(1,739)	1:136:B:LEU:HD23	1:137:B:PHE:H	4	0.28
(1,682)	1:110:B:ALA:H	1:112:B:GLU:H	17	0.28
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	5	0.28
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	4	0.28
(1,640)	1:92:B:THR:H	1:94:B:MET:H	10	0.28
(1,640)	1:92:B:THR:H	1:94:B:MET:H	14	0.28
(1,640)	1:92:B:THR:H	1:94:B:MET:H	20	0.28
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	18	0.28
(1,630)	1:87:B:ALA:H	1:89:B:ILE:H	16	0.28
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	14	0.28
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	5	0.28
(1,565)	1:60:B:LEU:H	1:82:B:GLY:H	14	0.28
(1,510)	1:47:B:ALA:H	1:61:B:ARG:H	14	0.28
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	13	0.28
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	6	0.28
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	6	0.28
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	6	0.28
(1,464)	1:32:B:PHE:H	1:34:B:LYS:H	12	0.28
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	12	0.28
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	19	0.28
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	16	0.28
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	9	0.28
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	1	0.28
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	1	0.28
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	7	0.28
(1,360)	1:122:A:THR:H	1:18:B:THR:H	14	0.28
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	19	0.28
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	16	0.28
(1,303)	1:97:A:CYS:H	1:98:A:LEU:H	2	0.28
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	16	0.28
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	16	0.28
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	16	0.28
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	1	0.28
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	19	0.28
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	19	0.28
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	10	0.28
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	10	0.28
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	4	0.28
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	11	0.28
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	15	0.28
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	17	0.28
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	18	0.28
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	4	0.28
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	4	0.28
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	18	0.28
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	5	0.27
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	5	0.27
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	5	0.27
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	5	0.27
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	5	0.27
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	5	0.27
(1,1647)	1:128:D:LEU:HD11	2:290:G:TRP:HE3	10	0.27
(1,1647)	1:128:D:LEU:HD12	2:290:G:TRP:HE3	10	0.27
(1,1647)	1:128:D:LEU:HD13	2:290:G:TRP:HE3	10	0.27
(1,1647)	1:128:D:LEU:HD21	2:290:G:TRP:HE3	10	0.27
(1,1647)	1:128:D:LEU:HD22	2:290:G:TRP:HE3	10	0.27
(1,1647)	1:128:D:LEU:HD23	2:290:G:TRP:HE3	10	0.27
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	8	0.27
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	8	0.27
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	8	0.27
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	8	0.27
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	8	0.27
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	8	0.27
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG21	6	0.27
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG22	6	0.27
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG23	6	0.27
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG21	6	0.27
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG22	6	0.27
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG23	6	0.27
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG21	6	0.27
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG22	6	0.27
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG23	6	0.27
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	15	0.27
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	15	0.27
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	15	0.27
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	15	0.27
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	15	0.27
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	15	0.27
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	15	0.27
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	15	0.27
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	6	0.27
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	6	0.27
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	6	0.27
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	6	0.27
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	6	0.27
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	6	0.27
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD11	18	0.27
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD12	18	0.27
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD13	18	0.27
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD21	18	0.27
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD22	18	0.27
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD23	18	0.27
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD11	18	0.27
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD12	18	0.27
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD13	18	0.27
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD21	18	0.27
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD22	18	0.27
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD23	18	0.27
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD11	18	0.27
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD12	18	0.27
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD13	18	0.27
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD21	18	0.27
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD22	18	0.27
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD23	18	0.27
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	4	0.27
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	7	0.27
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	2	0.27
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	8	0.27
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	8	0.27
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	8	0.27
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	1	0.27
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	7	0.27
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	13	0.27
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	20	0.27
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	20	0.27
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	13	0.27
(1,1088)	1:118:C:VAL:HG21	1:126:C:LEU:H	20	0.27
(1,1088)	1:118:C:VAL:HG22	1:126:C:LEU:H	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1088)	1:118:C:VAL:HG23	1:126:C:LEU:H	20	0.27
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	7	0.27
(1,1050)	1:99:C:GLY:H	1:102:C:CYS:H	16	0.27
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	19	0.27
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	17	0.27
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	17	0.27
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	20	0.27
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	4	0.27
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	13	0.27
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	14	0.27
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	8	0.27
(1,840)	1:36:C:TRP:H	1:37:C:GLN:H	19	0.27
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	5	0.27
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	18	0.27
(1,800)	1:22:C:SER:H	1:79:C:GLN:H	6	0.27
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	2	0.27
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	8	0.27
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	8	0.27
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD1	1	0.27
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD2	1	0.27
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD1	1	0.27
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD2	1	0.27
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD1	1	0.27
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD2	1	0.27
(1,670)	1:100:B:ALA:H	1:101:B:TYR:H	3	0.27
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	1	0.27
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	6	0.27
(1,647)	1:94:B:MET:H	1:97:B:CYS:H	19	0.27
(1,641)	1:92:B:THR:H	1:95:B:ALA:H	14	0.27
(1,640)	1:92:B:THR:H	1:94:B:MET:H	7	0.27
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	9	0.27
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	16	0.27
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB1	17	0.27
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB2	17	0.27
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB3	17	0.27
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	17	0.27
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	8	0.27
(1,523)	1:51:B:LEU:HD21	1:57:B:GLU:H	1	0.27
(1,523)	1:51:B:LEU:HD22	1:57:B:GLU:H	1	0.27
(1,523)	1:51:B:LEU:HD23	1:57:B:GLU:H	1	0.27
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	12	0.27
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	11	0.27
(1,464)	1:32:B:PHE:H	1:34:B:LYS:H	18	0.27
(1,441)	1:23:B:PHE:H	1:24:B:GLU:H	16	0.27
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	9	0.27
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	9	0.27
(1,403)	1:9:B:MET:HE1	1:10:B:THR:H	4	0.27
(1,403)	1:9:B:MET:HE2	1:10:B:THR:H	4	0.27
(1,403)	1:9:B:MET:HE3	1:10:B:THR:H	4	0.27
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	1	0.27
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	10	0.27
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	11	0.27
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	11	0.27
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	17	0.27
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	19	0.27
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	1	0.27
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	9	0.27
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	13	0.27
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	4	0.27
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD21	4	0.27
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD22	4	0.27
(1,96)	1:37:A:GLN:H	1:68:A:LEU:HD23	4	0.27
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	20	0.27
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	20	0.27
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	20	0.27
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	8	0.27
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	14	0.27
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD11	20	0.26
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD12	20	0.26
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD13	20	0.26
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD11	20	0.26
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD12	20	0.26
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD13	20	0.26
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD11	20	0.26
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD12	20	0.26
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD13	20	0.26
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	20	0.26
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	20	0.26
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	20	0.26
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	20	0.26
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	20	0.26
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	20	0.26
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	13	0.26
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	13	0.26
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	15	0.26
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	15	0.26
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	15	0.26
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	15	0.26
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	15	0.26
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	15	0.26
(1,1647)	1:128:D:LEU:HD11	2:290:G:TRP:HE3	15	0.26
(1,1647)	1:128:D:LEU:HD12	2:290:G:TRP:HE3	15	0.26
(1,1647)	1:128:D:LEU:HD13	2:290:G:TRP:HE3	15	0.26
(1,1647)	1:128:D:LEU:HD21	2:290:G:TRP:HE3	15	0.26
(1,1647)	1:128:D:LEU:HD22	2:290:G:TRP:HE3	15	0.26
(1,1647)	1:128:D:LEU:HD23	2:290:G:TRP:HE3	15	0.26
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD11	10	0.26
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD12	10	0.26
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD13	10	0.26
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD21	10	0.26
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD22	10	0.26
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD23	10	0.26
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD11	10	0.26
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD12	10	0.26
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD13	10	0.26
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD21	10	0.26
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD22	10	0.26
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD23	10	0.26
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD11	10	0.26
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD12	10	0.26
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD13	10	0.26
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD21	10	0.26
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD22	10	0.26
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD23	10	0.26
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD11	10	0.26
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD12	10	0.26
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD13	10	0.26
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD21	10	0.26
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD22	10	0.26
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD23	10	0.26
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD11	10	0.26
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD12	10	0.26
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD13	10	0.26
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD21	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD22	10	0.26
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD23	10	0.26
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD11	10	0.26
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD12	10	0.26
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD13	10	0.26
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD21	10	0.26
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD22	10	0.26
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD23	10	0.26
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE1	5	0.26
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE2	5	0.26
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE1	5	0.26
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE2	5	0.26
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG21	19	0.26
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG22	19	0.26
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG23	19	0.26
(1,1469)	1:133:D:PHE:H	1:135:D:ALA:H	2	0.26
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	4	0.26
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	3	0.26
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	14	0.26
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	11	0.26
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	11	0.26
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	11	0.26
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	12	0.26
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	12	0.26
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	12	0.26
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	11	0.26
(1,1198)	1:31:D:VAL:HG21	1:72:D:THR:H	9	0.26
(1,1198)	1:31:D:VAL:HG22	1:72:D:THR:H	9	0.26
(1,1198)	1:31:D:VAL:HG23	1:72:D:THR:H	9	0.26
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	16	0.26
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	9	0.26
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	12	0.26
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	13	0.26
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	5	0.26
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE1	12	0.26
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE2	12	0.26
(1,917)	1:56:C:TYR:HE1	1:94:C:MET:HE3	12	0.26
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE1	12	0.26
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE2	12	0.26
(1,917)	1:56:C:TYR:HE2	1:94:C:MET:HE3	12	0.26
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	14	0.26
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:45:C:ASP:H	1:63:C:THR:H	13	0.26
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	1	0.26
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	8	0.26
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	12	0.26
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	3	0.26
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	8	0.26
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	18	0.26
(1,750)	1:139:B:ASN:H	1:141:B:LEU:H	2	0.26
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	16	0.26
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	16	0.26
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	16	0.26
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	9	0.26
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	18	0.26
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	5	0.26
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	18	0.26
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	1	0.26
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	13	0.26
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	10	0.26
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	16	0.26
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	1	0.26
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	12	0.26
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG21	1	0.26
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG22	1	0.26
(1,568)	1:60:B:LEU:HD21	1:62:B:VAL:HG23	1	0.26
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG21	1	0.26
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG22	1	0.26
(1,568)	1:60:B:LEU:HD22	1:62:B:VAL:HG23	1	0.26
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG21	1	0.26
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG22	1	0.26
(1,568)	1:60:B:LEU:HD23	1:62:B:VAL:HG23	1	0.26
(1,523)	1:51:B:LEU:HD21	1:57:B:GLU:H	6	0.26
(1,523)	1:51:B:LEU:HD22	1:57:B:GLU:H	6	0.26
(1,523)	1:51:B:LEU:HD23	1:57:B:GLU:H	6	0.26
(1,416)	1:13:B:ILE:H	1:129:D:ALA:HB1	16	0.26
(1,416)	1:13:B:ILE:H	1:129:D:ALA:HB2	16	0.26
(1,416)	1:13:B:ILE:H	1:129:D:ALA:HB3	16	0.26
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	16	0.26
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD21	18	0.26
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD22	18	0.26
(1,375)	1:131:A:VAL:HG21	1:136:A:LEU:HD23	18	0.26
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD21	18	0.26
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD22	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:131:A:VAL:HG22	1:136:A:LEU:HD23	18	0.26
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD21	18	0.26
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD22	18	0.26
(1,375)	1:131:A:VAL:HG23	1:136:A:LEU:HD23	18	0.26
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE1	19	0.26
(1,374)	1:131:A:VAL:HG11	1:133:A:PHE:HE2	19	0.26
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE1	19	0.26
(1,374)	1:131:A:VAL:HG12	1:133:A:PHE:HE2	19	0.26
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE1	19	0.26
(1,374)	1:131:A:VAL:HG13	1:133:A:PHE:HE2	19	0.26
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	18	0.26
(1,357)	1:121:A:GLY:H	1:123:A:PHE:H	2	0.26
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	4	0.26
(1,284)	1:92:A:THR:H	1:93:A:GLN:H	5	0.26
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	5	0.26
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD1	6	0.26
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD2	6	0.26
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	10	0.26
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	12	0.26
(1,130)	1:45:A:ASP:H	1:61:A:ARG:H	2	0.26
(1,123)	1:44:A:LEU:HD11	1:45:A:ASP:H	16	0.26
(1,123)	1:44:A:LEU:HD12	1:45:A:ASP:H	16	0.26
(1,123)	1:44:A:LEU:HD13	1:45:A:ASP:H	16	0.26
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	2	0.26
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	3	0.26
(1,120)	1:43:A:ASP:H	1:65:A:THR:H	20	0.26
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	4	0.26
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	6	0.26
(1,1694)	1:42:B:LEU:HD11	2:291:H:LEU:HD11	16	0.25
(1,1694)	1:42:B:LEU:HD11	2:291:H:LEU:HD12	16	0.25
(1,1694)	1:42:B:LEU:HD11	2:291:H:LEU:HD13	16	0.25
(1,1694)	1:42:B:LEU:HD12	2:291:H:LEU:HD11	16	0.25
(1,1694)	1:42:B:LEU:HD12	2:291:H:LEU:HD12	16	0.25
(1,1694)	1:42:B:LEU:HD12	2:291:H:LEU:HD13	16	0.25
(1,1694)	1:42:B:LEU:HD13	2:291:H:LEU:HD11	16	0.25
(1,1694)	1:42:B:LEU:HD13	2:291:H:LEU:HD12	16	0.25
(1,1694)	1:42:B:LEU:HD13	2:291:H:LEU:HD13	16	0.25
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	19	0.25
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	19	0.25
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	19	0.25
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	1	0.25
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	1	0.25
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	1	0.25
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	1	0.25
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	1	0.25
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG21	2	0.25
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG22	2	0.25
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG23	2	0.25
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG21	2	0.25
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG22	2	0.25
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG23	2	0.25
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG21	2	0.25
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG22	2	0.25
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG23	2	0.25
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	4	0.25
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	4	0.25
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	4	0.25
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	4	0.25
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	4	0.25
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	4	0.25
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	4	0.25
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	4	0.25
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	4	0.25
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	4	0.25
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	4	0.25
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	4	0.25
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	9	0.25
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	9	0.25
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	9	0.25
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	9	0.25
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	9	0.25
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	9	0.25
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	19	0.25
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	19	0.25
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	19	0.25
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	19	0.25
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	19	0.25
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	19	0.25
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	16	0.25
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	16	0.25
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	16	0.25
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	16	0.25
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	16	0.25
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	16	0.25
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	16	0.25
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	16	0.25
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	16	0.25
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	16	0.25
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	16	0.25
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	16	0.25
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	16	0.25
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	16	0.25
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	16	0.25
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	16	0.25
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	16	0.25
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	17	0.25
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG21	6	0.25
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG22	6	0.25
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG23	6	0.25
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG21	6	0.25
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG22	6	0.25
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG23	6	0.25
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG21	6	0.25
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG22	6	0.25
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG23	6	0.25
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG21	12	0.25
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG22	12	0.25
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG23	12	0.25
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG21	12	0.25
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG22	12	0.25
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG23	12	0.25
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG21	12	0.25
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG22	12	0.25
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG23	12	0.25
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	1	0.25
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	3	0.25
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	12	0.25
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	18	0.25
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	20	0.25
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	4	0.25
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	13	0.25
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	16	0.25
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	10	0.25
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	10	0.25
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	3	0.25
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	3	0.25
(1,1111)	1:133:C:PHE:H	1:134:C:ASP:H	6	0.25
(1,1088)	1:118:C:VAL:HG21	1:126:C:LEU:H	15	0.25
(1,1088)	1:118:C:VAL:HG22	1:126:C:LEU:H	15	0.25
(1,1088)	1:118:C:VAL:HG23	1:126:C:LEU:H	15	0.25
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	13	0.25
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	15	0.25
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	3	0.25
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	6	0.25
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD21	10	0.25
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD22	10	0.25
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD23	10	0.25
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	8	0.25
(1,840)	1:36:C:TRP:H	1:37:C:GLN:H	14	0.25
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	13	0.25
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	7	0.25
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	10	0.25
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	10	0.25
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	10	0.25
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	14	0.25
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	14	0.25
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	20	0.25
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	2	0.25
(1,498)	1:44:B:LEU:H	1:63:B:THR:H	6	0.25
(1,498)	1:44:B:LEU:H	1:63:B:THR:H	17	0.25
(1,496)	1:43:B:ASP:H	1:65:B:THR:H	13	0.25
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	12	0.25
(1,466)	1:33:B:GLN:H	1:34:B:LYS:H	13	0.25
(1,441)	1:23:B:PHE:H	1:24:B:GLU:H	4	0.25
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	17	0.25
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	9	0.25
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	8	0.25
(1,400)	1:140:A:TYR:H	1:141:A:LEU:H	4	0.25
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	4	0.25
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	3	0.25
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	13	0.25
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	17	0.25
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	18	0.25
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	10	0.25
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:95:A:ALA:H	1:98:A:LEU:H	19	0.25
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	11	0.25
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	17	0.25
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	17	0.25
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	17	0.25
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	20	0.25
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	20	0.25
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	20	0.25
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	5	0.25
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	16	0.25
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	4	0.25
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	14	0.25
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD1	20	0.25
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD2	20	0.25
(1,136)	1:47:A:ALA:H	1:59:A:VAL:H	6	0.25
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	7	0.25
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	11	0.25
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	11	0.25
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	11	0.25
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	19	0.25
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	7	0.25
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	10	0.25
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	10	0.25
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	14	0.25
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	10	0.25
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	8	0.25
(2,1)	1:40:A:VAL:O	2:290:E:TRP:NE1	20	0.24
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	3	0.24
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	3	0.24
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	3	0.24
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	3	0.24
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	3	0.24
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	3	0.24
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD11	8	0.24
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD12	8	0.24
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD13	8	0.24
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD11	8	0.24
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD12	8	0.24
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD13	8	0.24
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD11	8	0.24
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD12	8	0.24
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD13	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	14	0.24
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	14	0.24
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	14	0.24
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	19	0.24
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	19	0.24
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	19	0.24
(1,1668)	1:40:B:VAL:HG11	2:290:H:TRP:HE1	11	0.24
(1,1668)	1:40:B:VAL:HG12	2:290:H:TRP:HE1	11	0.24
(1,1668)	1:40:B:VAL:HG13	2:290:H:TRP:HE1	11	0.24
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	8	0.24
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	8	0.24
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	8	0.24
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	8	0.24
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	8	0.24
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	8	0.24
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	8	0.24
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	8	0.24
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	8	0.24
(1,1637)	1:98:D:LEU:HD11	2:281:G:PHE:HZ	18	0.24
(1,1637)	1:98:D:LEU:HD12	2:281:G:PHE:HZ	18	0.24
(1,1637)	1:98:D:LEU:HD13	2:281:G:PHE:HZ	18	0.24
(1,1637)	1:98:D:LEU:HD21	2:281:G:PHE:HZ	18	0.24
(1,1637)	1:98:D:LEU:HD22	2:281:G:PHE:HZ	18	0.24
(1,1637)	1:98:D:LEU:HD23	2:281:G:PHE:HZ	18	0.24
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD11	7	0.24
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD12	7	0.24
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD13	7	0.24
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD21	7	0.24
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD22	7	0.24
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD23	7	0.24
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD11	7	0.24
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD12	7	0.24
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD13	7	0.24
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD21	7	0.24
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD22	7	0.24
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD23	7	0.24
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD11	7	0.24
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD12	7	0.24
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD13	7	0.24
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD21	7	0.24
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD22	7	0.24
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD23	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE1	9	0.24
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE2	9	0.24
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE1	9	0.24
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE2	9	0.24
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	16	0.24
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	16	0.24
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	16	0.24
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	20	0.24
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	20	0.24
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	20	0.24
(1,1597)	1:129:B:ALA:HB1	2:306:F:VAL:HG11	16	0.24
(1,1597)	1:129:B:ALA:HB1	2:306:F:VAL:HG12	16	0.24
(1,1597)	1:129:B:ALA:HB1	2:306:F:VAL:HG13	16	0.24
(1,1597)	1:129:B:ALA:HB2	2:306:F:VAL:HG11	16	0.24
(1,1597)	1:129:B:ALA:HB2	2:306:F:VAL:HG12	16	0.24
(1,1597)	1:129:B:ALA:HB2	2:306:F:VAL:HG13	16	0.24
(1,1597)	1:129:B:ALA:HB3	2:306:F:VAL:HG11	16	0.24
(1,1597)	1:129:B:ALA:HB3	2:306:F:VAL:HG12	16	0.24
(1,1597)	1:129:B:ALA:HB3	2:306:F:VAL:HG13	16	0.24
(1,1594)	1:128:C:LEU:HD11	2:290:F:TRP:HE3	19	0.24
(1,1594)	1:128:C:LEU:HD12	2:290:F:TRP:HE3	19	0.24
(1,1594)	1:128:C:LEU:HD13	2:290:F:TRP:HE3	19	0.24
(1,1594)	1:128:C:LEU:HD21	2:290:F:TRP:HE3	19	0.24
(1,1594)	1:128:C:LEU:HD22	2:290:F:TRP:HE3	19	0.24
(1,1594)	1:128:C:LEU:HD23	2:290:F:TRP:HE3	19	0.24
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	6	0.24
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	6	0.24
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	6	0.24
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	6	0.24
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	6	0.24
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	6	0.24
(1,1541)	1:128:A:LEU:HD11	2:290:E:TRP:HE3	8	0.24
(1,1541)	1:128:A:LEU:HD12	2:290:E:TRP:HE3	8	0.24
(1,1541)	1:128:A:LEU:HD13	2:290:E:TRP:HE3	8	0.24
(1,1541)	1:128:A:LEU:HD21	2:290:E:TRP:HE3	8	0.24
(1,1541)	1:128:A:LEU:HD22	2:290:E:TRP:HE3	8	0.24
(1,1541)	1:128:A:LEU:HD23	2:290:E:TRP:HE3	8	0.24
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD11	15	0.24
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD12	15	0.24
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD13	15	0.24
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD21	15	0.24
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD22	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD23	15	0.24
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD11	15	0.24
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD12	15	0.24
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD13	15	0.24
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD21	15	0.24
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD22	15	0.24
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD23	15	0.24
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD11	15	0.24
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD12	15	0.24
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD13	15	0.24
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD21	15	0.24
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD22	15	0.24
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD23	15	0.24
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD11	15	0.24
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD12	15	0.24
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD13	15	0.24
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD21	15	0.24
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD22	15	0.24
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD23	15	0.24
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD11	15	0.24
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD12	15	0.24
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD13	15	0.24
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD21	15	0.24
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD22	15	0.24
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD23	15	0.24
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD11	15	0.24
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD12	15	0.24
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD13	15	0.24
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD21	15	0.24
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD22	15	0.24
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD23	15	0.24
(1,1462)	1:128:D:LEU:HD11	1:129:D:ALA:H	7	0.24
(1,1462)	1:128:D:LEU:HD12	1:129:D:ALA:H	7	0.24
(1,1462)	1:128:D:LEU:HD13	1:129:D:ALA:H	7	0.24
(1,1458)	1:126:D:LEU:H	1:127:D:ASN:H	20	0.24
(1,1412)	1:99:D:GLY:H	1:102:D:CYS:H	8	0.24
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	16	0.24
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	16	0.24
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	19	0.24
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	7	0.24
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	14	0.24
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	7	0.24
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	9	0.24
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	10	0.24
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	5	0.24
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	3	0.24
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	3	0.24
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	3	0.24
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	7	0.24
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	7	0.24
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	7	0.24
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	14	0.24
(1,1171)	1:23:D:PHE:HE1	1:24:D:GLU:H	9	0.24
(1,1171)	1:23:D:PHE:HE2	1:24:D:GLU:H	9	0.24
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	17	0.24
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	6	0.24
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	15	0.24
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	9	0.24
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	9	0.24
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	9	0.24
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	16	0.24
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	17	0.24
(1,1045)	1:98:C:LEU:H	1:102:C:CYS:H	8	0.24
(1,1042)	1:98:C:LEU:H	1:99:C:GLY:H	9	0.24
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	12	0.24
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	17	0.24
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	7	0.24
(1,875)	1:45:C:ASP:H	1:61:C:ARG:H	19	0.24
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	11	0.24
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	6	0.24
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	6	0.24
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	6	0.24
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	12	0.24
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	15	0.24
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD1	15	0.24
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD2	15	0.24
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD1	15	0.24
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD2	15	0.24
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD1	15	0.24
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD2	15	0.24
(1,706)	1:118:B:VAL:HG11	1:126:B:LEU:H	14	0.24
(1,706)	1:118:B:VAL:HG12	1:126:B:LEU:H	14	0.24
(1,706)	1:118:B:VAL:HG13	1:126:B:LEU:H	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	13	0.24
(1,658)	1:97:B:CYS:H	1:99:B:GLY:H	10	0.24
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	20	0.24
(1,640)	1:92:B:THR:H	1:94:B:MET:H	18	0.24
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	13	0.24
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	7	0.24
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	19	0.24
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	3	0.24
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	8	0.24
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	4	0.24
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	15	0.24
(1,594)	1:68:B:LEU:H	1:71:B:GLU:H	7	0.24
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	9	0.24
(1,523)	1:51:B:LEU:HD21	1:57:B:GLU:H	3	0.24
(1,523)	1:51:B:LEU:HD22	1:57:B:GLU:H	3	0.24
(1,523)	1:51:B:LEU:HD23	1:57:B:GLU:H	3	0.24
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	1	0.24
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	13	0.24
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	19	0.24
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD11	4	0.24
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD12	4	0.24
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD13	4	0.24
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD11	4	0.24
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD12	4	0.24
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD13	4	0.24
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD11	4	0.24
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD12	4	0.24
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD13	4	0.24
(1,499)	1:44:B:LEU:HD11	1:45:B:ASP:H	12	0.24
(1,499)	1:44:B:LEU:HD12	1:45:B:ASP:H	12	0.24
(1,499)	1:44:B:LEU:HD13	1:45:B:ASP:H	12	0.24
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	10	0.24
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	19	0.24
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	20	0.24
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	6	0.24
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	6	0.24
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	1	0.24
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	2	0.24
(1,369)	1:128:A:LEU:HD11	1:129:A:ALA:HB1	12	0.24
(1,369)	1:128:A:LEU:HD11	1:129:A:ALA:HB2	12	0.24
(1,369)	1:128:A:LEU:HD11	1:129:A:ALA:HB3	12	0.24
(1,369)	1:128:A:LEU:HD12	1:129:A:ALA:HB1	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:128:A:LEU:HD12	1:129:A:ALA:HB2	12	0.24
(1,369)	1:128:A:LEU:HD12	1:129:A:ALA:HB3	12	0.24
(1,369)	1:128:A:LEU:HD13	1:129:A:ALA:HB1	12	0.24
(1,369)	1:128:A:LEU:HD13	1:129:A:ALA:HB2	12	0.24
(1,369)	1:128:A:LEU:HD13	1:129:A:ALA:HB3	12	0.24
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	5	0.24
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	18	0.24
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	8	0.24
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	7	0.24
(1,303)	1:97:A:CYS:H	1:98:A:LEU:H	18	0.24
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	1	0.24
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	9	0.24
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	10	0.24
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	1	0.24
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	1	0.24
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	1	0.24
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	14	0.24
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	14	0.24
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	14	0.24
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	18	0.24
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	18	0.24
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	18	0.24
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE1	7	0.24
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE2	7	0.24
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE3	7	0.24
(1,237)	1:70:A:GLU:H	1:71:A:GLU:H	18	0.24
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	19	0.24
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	15	0.24
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	16	0.24
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG21	15	0.24
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG22	15	0.24
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG23	15	0.24
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG21	15	0.24
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG22	15	0.24
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG23	15	0.24
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG21	15	0.24
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG22	15	0.24
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG23	15	0.24
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	6	0.24
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	11	0.24
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	12	0.24
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	5	0.24
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	16	0.24
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	16	0.24
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	2	0.24
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	1	0.24
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	3	0.24
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	11	0.23
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG21	12	0.23
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG22	12	0.23
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG23	12	0.23
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG21	12	0.23
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG22	12	0.23
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG23	12	0.23
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG21	12	0.23
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG22	12	0.23
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG23	12	0.23
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD11	6	0.23
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD12	6	0.23
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD13	6	0.23
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD11	6	0.23
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD12	6	0.23
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD13	6	0.23
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD11	6	0.23
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD12	6	0.23
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD13	6	0.23
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	7	0.23
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	7	0.23
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	7	0.23
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD11	18	0.23
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD12	18	0.23
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD13	18	0.23
(1,1647)	1:128:D:LEU:HD11	2:290:G:TRP:HE3	6	0.23
(1,1647)	1:128:D:LEU:HD12	2:290:G:TRP:HE3	6	0.23
(1,1647)	1:128:D:LEU:HD13	2:290:G:TRP:HE3	6	0.23
(1,1647)	1:128:D:LEU:HD21	2:290:G:TRP:HE3	6	0.23
(1,1647)	1:128:D:LEU:HD22	2:290:G:TRP:HE3	6	0.23
(1,1647)	1:128:D:LEU:HD23	2:290:G:TRP:HE3	6	0.23
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD11	9	0.23
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD12	9	0.23
(1,1620)	1:123:D:PHE:HE1	2:301:G:ILE:HD13	9	0.23
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD11	9	0.23
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD12	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1620)	1:123:D:PHE:HE2	2:301:G:ILE:HD13	9	0.23
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG21	12	0.23
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG22	12	0.23
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG23	12	0.23
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG21	12	0.23
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG22	12	0.23
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG23	12	0.23
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG21	12	0.23
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG22	12	0.23
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG23	12	0.23
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD11	1	0.23
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD12	1	0.23
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD13	1	0.23
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD21	1	0.23
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD22	1	0.23
(1,1577)	1:86:C:ILE:HD11	2:278:F:LEU:HD23	1	0.23
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD11	1	0.23
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD12	1	0.23
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD13	1	0.23
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD21	1	0.23
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD22	1	0.23
(1,1577)	1:86:C:ILE:HD12	2:278:F:LEU:HD23	1	0.23
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD11	1	0.23
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD12	1	0.23
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD13	1	0.23
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD21	1	0.23
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD22	1	0.23
(1,1577)	1:86:C:ILE:HD13	2:278:F:LEU:HD23	1	0.23
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD11	13	0.23
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD12	13	0.23
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD13	13	0.23
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD11	13	0.23
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD12	13	0.23
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD13	13	0.23
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE1	18	0.23
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE2	18	0.23
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE3	18	0.23
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE1	18	0.23
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE2	18	0.23
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE3	18	0.23
(1,1469)	1:133:D:PHE:H	1:135:D:ALA:H	10	0.23
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1412)	1:99:D:GLY:H	1:102:D:CYS:H	15	0.23
(1,1394)	1:94:D:MET:HE1	1:98:D:LEU:H	9	0.23
(1,1394)	1:94:D:MET:HE2	1:98:D:LEU:H	9	0.23
(1,1394)	1:94:D:MET:HE3	1:98:D:LEU:H	9	0.23
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	1	0.23
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	19	0.23
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	8	0.23
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	10	0.23
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	15	0.23
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	8	0.23
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	17	0.23
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	6	0.23
(1,1206)	1:35:D:ASP:H	1:36:D:TRP:HE3	10	0.23
(1,1186)	1:30:D:HIS:H	1:32:D:PHE:H	16	0.23
(1,1155)	1:17:D:TYR:H	1:81:D:GLY:H	16	0.23
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	1	0.23
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	1	0.23
(1,1118)	1:135:C:ALA:H	1:138:C:MET:H	10	0.23
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	17	0.23
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	17	0.23
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	17	0.23
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	12	0.23
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	12	0.23
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	12	0.23
(1,1095)	1:122:C:THR:H	1:18:D:THR:H	13	0.23
(1,1093)	1:121:C:GLY:H	1:18:D:THR:H	13	0.23
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	1	0.23
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	8	0.23
(1,995)	1:77:C:GLU:H	1:78:C:VAL:H	19	0.23
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	4	0.23
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	12	0.23
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	17	0.23
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD21	16	0.23
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD22	16	0.23
(1,847)	1:39:C:GLU:H	1:68:C:LEU:HD23	16	0.23
(1,840)	1:36:C:TRP:H	1:37:C:GLN:H	2	0.23
(1,840)	1:36:C:TRP:H	1:37:C:GLN:H	16	0.23
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	5	0.23
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	1	0.23
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	1	0.23
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	1	0.23
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	8	0.23
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	19	0.23
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	18	0.23
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	9	0.23
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	10	0.23
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	13	0.23
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	1	0.23
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	6	0.23
(1,630)	1:87:B:ALA:H	1:89:B:ILE:H	12	0.23
(1,594)	1:68:B:LEU:H	1:71:B:GLU:H	13	0.23
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	7	0.23
(1,581)	1:64:B:VAL:HG21	1:128:B:LEU:HD11	3	0.23
(1,581)	1:64:B:VAL:HG21	1:128:B:LEU:HD12	3	0.23
(1,581)	1:64:B:VAL:HG21	1:128:B:LEU:HD13	3	0.23
(1,581)	1:64:B:VAL:HG22	1:128:B:LEU:HD11	3	0.23
(1,581)	1:64:B:VAL:HG22	1:128:B:LEU:HD12	3	0.23
(1,581)	1:64:B:VAL:HG22	1:128:B:LEU:HD13	3	0.23
(1,581)	1:64:B:VAL:HG23	1:128:B:LEU:HD11	3	0.23
(1,581)	1:64:B:VAL:HG23	1:128:B:LEU:HD12	3	0.23
(1,581)	1:64:B:VAL:HG23	1:128:B:LEU:HD13	3	0.23
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	19	0.23
(1,565)	1:60:B:LEU:H	1:82:B:GLY:H	3	0.23
(1,521)	1:51:B:LEU:H	1:57:B:GLU:H	1	0.23
(1,506)	1:45:B:ASP:H	1:63:B:THR:H	10	0.23
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD21	15	0.23
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD22	15	0.23
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD23	15	0.23
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	8	0.23
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	3	0.23
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	18	0.23
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	4	0.23
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	7	0.23
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	2	0.23
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	18	0.23
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	13	0.23
(1,370)	1:128:A:LEU:HD21	1:129:A:ALA:H	20	0.23
(1,370)	1:128:A:LEU:HD22	1:129:A:ALA:H	20	0.23
(1,370)	1:128:A:LEU:HD23	1:129:A:ALA:H	20	0.23
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	14	0.23
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	14	0.23
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	20	0.23
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	19	0.23
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	7	0.23
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	4	0.23
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	4	0.23
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	5	0.23
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	5	0.23
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	5	0.23
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	15	0.23
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	15	0.23
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	15	0.23
(1,229)	1:68:A:LEU:H	1:69:A:GLY:H	11	0.23
(1,192)	1:60:A:LEU:H	1:81:A:GLY:H	19	0.23
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	1	0.23
(1,146)	1:50:A:GLN:H	1:57:A:GLU:H	15	0.23
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	7	0.23
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	20	0.23
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	20	0.23
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	20	0.23
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	10	0.23
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	11	0.23
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	10	0.22
(1,1700)	1:128:B:LEU:HD11	2:290:H:TRP:HE3	4	0.22
(1,1700)	1:128:B:LEU:HD12	2:290:H:TRP:HE3	4	0.22
(1,1700)	1:128:B:LEU:HD13	2:290:H:TRP:HE3	4	0.22
(1,1700)	1:128:B:LEU:HD21	2:290:H:TRP:HE3	4	0.22
(1,1700)	1:128:B:LEU:HD22	2:290:H:TRP:HE3	4	0.22
(1,1700)	1:128:B:LEU:HD23	2:290:H:TRP:HE3	4	0.22
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	14	0.22
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	14	0.22
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	14	0.22
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	14	0.22
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	14	0.22
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	14	0.22
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD11	4	0.22
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD12	4	0.22
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD13	4	0.22
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD21	4	0.22
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD22	4	0.22
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD23	4	0.22
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD11	4	0.22
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD12	4	0.22
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD13	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD21	4	0.22
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD22	4	0.22
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD23	4	0.22
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD11	4	0.22
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD12	4	0.22
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD13	4	0.22
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD21	4	0.22
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD22	4	0.22
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD23	4	0.22
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	12	0.22
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	12	0.22
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	12	0.22
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	12	0.22
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	12	0.22
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	12	0.22
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	12	0.22
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	12	0.22
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	12	0.22
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	9	0.22
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	9	0.22
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	9	0.22
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	9	0.22
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	9	0.22
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	9	0.22
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD11	10	0.22
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD12	10	0.22
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD13	10	0.22
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD11	10	0.22
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD12	10	0.22
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD13	10	0.22
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD11	10	0.22
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD12	10	0.22
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD13	10	0.22
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD11	18	0.22
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD12	18	0.22
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD13	18	0.22
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD21	18	0.22
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD22	18	0.22
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD23	18	0.22
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD11	18	0.22
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD12	18	0.22
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD13	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD21	18	0.22
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD22	18	0.22
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD23	18	0.22
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD11	18	0.22
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD12	18	0.22
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD13	18	0.22
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD21	18	0.22
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD22	18	0.22
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD23	18	0.22
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD11	18	0.22
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD12	18	0.22
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD13	18	0.22
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD21	18	0.22
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD22	18	0.22
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD23	18	0.22
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD11	18	0.22
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD12	18	0.22
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD13	18	0.22
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD21	18	0.22
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD22	18	0.22
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD23	18	0.22
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD11	18	0.22
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD12	18	0.22
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD13	18	0.22
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD21	18	0.22
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD22	18	0.22
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD23	18	0.22
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	5	0.22
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	5	0.22
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	5	0.22
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	5	0.22
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	5	0.22
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	5	0.22
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	5	0.22
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	5	0.22
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	5	0.22
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	8	0.22
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	8	0.22
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	8	0.22
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	8	0.22
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	8	0.22
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	8	0.22
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	8	0.22
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	8	0.22
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD21	19	0.22
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD22	19	0.22
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD23	19	0.22
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD21	19	0.22
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD22	19	0.22
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD23	19	0.22
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD21	19	0.22
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD22	19	0.22
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD23	19	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	6	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	6	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	6	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	8	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	8	0.22
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	8	0.22
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG21	16	0.22
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG22	16	0.22
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG23	16	0.22
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG21	16	0.22
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG22	16	0.22
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG23	16	0.22
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG21	16	0.22
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG22	16	0.22
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG23	16	0.22
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG21	20	0.22
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG22	20	0.22
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG23	20	0.22
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG21	20	0.22
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG22	20	0.22
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG23	20	0.22
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG21	20	0.22
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG22	20	0.22
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG23	20	0.22
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	13	0.22
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	13	0.22
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	13	0.22
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	13	0.22
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	13	0.22
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD11	19	0.22
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD12	19	0.22
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD13	19	0.22
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD21	19	0.22
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD22	19	0.22
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD23	19	0.22
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD11	19	0.22
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD12	19	0.22
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD13	19	0.22
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD21	19	0.22
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD22	19	0.22
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD23	19	0.22
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD11	19	0.22
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD12	19	0.22
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD13	19	0.22
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD21	19	0.22
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD22	19	0.22
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD23	19	0.22
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	6	0.22
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	6	0.22
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	6	0.22
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	6	0.22
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	6	0.22
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	6	0.22
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	6	0.22
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	6	0.22
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	6	0.22
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	6	0.22
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	6	0.22
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	6	0.22
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	6	0.22
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	6	0.22
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	6	0.22
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	6	0.22
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	6	0.22
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	6	0.22
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	14	0.22
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	8	0.22
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	11	0.22
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	8	0.22
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	6	0.22
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	11	0.22
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	6	0.22
(1,1176)	1:24:D:GLU:H	1:75:D:LEU:H	8	0.22
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	18	0.22
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	4	0.22
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	18	0.22
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	18	0.22
(1,1118)	1:135:C:ALA:H	1:138:C:MET:H	18	0.22
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	11	0.22
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	11	0.22
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	11	0.22
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	20	0.22
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	6	0.22
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	3	0.22
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	7	0.22
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	9	0.22
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	15	0.22
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD1	7	0.22
(1,988)	1:74:C:PHE:HE1	1:123:C:PHE:HD2	7	0.22
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD1	7	0.22
(1,988)	1:74:C:PHE:HE2	1:123:C:PHE:HD2	7	0.22
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	5	0.22
(1,960)	1:66:C:ALA:H	1:67:C:SER:H	9	0.22
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD21	20	0.22
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD22	20	0.22
(1,926)	1:58:C:VAL:HG11	1:98:C:LEU:HD23	20	0.22
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD21	20	0.22
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD22	20	0.22
(1,926)	1:58:C:VAL:HG12	1:98:C:LEU:HD23	20	0.22
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD21	20	0.22
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD22	20	0.22
(1,926)	1:58:C:VAL:HG13	1:98:C:LEU:HD23	20	0.22
(1,922)	1:58:C:VAL:H	1:84:C:PHE:H	13	0.22
(1,922)	1:58:C:VAL:H	1:84:C:PHE:H	20	0.22
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	14	0.22
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	18	0.22
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	12	0.22
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	12	0.22
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG11	11	0.22
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG12	11	0.22
(1,853)	1:41:C:LYS:H	1:64:C:VAL:HG13	11	0.22
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB1	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB2	9	0.22
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB3	9	0.22
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	1	0.22
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	1	0.22
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	1	0.22
(1,821)	1:30:C:HIS:H	1:32:C:PHE:H	11	0.22
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE1	15	0.22
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE2	15	0.22
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE1	15	0.22
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE2	15	0.22
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE1	15	0.22
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE2	15	0.22
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	8	0.22
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	11	0.22
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	19	0.22
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	19	0.22
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB1	6	0.22
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB2	6	0.22
(1,723)	1:128:B:LEU:HD21	1:129:B:ALA:HB3	6	0.22
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB1	6	0.22
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB2	6	0.22
(1,723)	1:128:B:LEU:HD22	1:129:B:ALA:HB3	6	0.22
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB1	6	0.22
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB2	6	0.22
(1,723)	1:128:B:LEU:HD23	1:129:B:ALA:HB3	6	0.22
(1,706)	1:118:B:VAL:HG11	1:126:B:LEU:H	19	0.22
(1,706)	1:118:B:VAL:HG12	1:126:B:LEU:H	19	0.22
(1,706)	1:118:B:VAL:HG13	1:126:B:LEU:H	19	0.22
(1,682)	1:110:B:ALA:H	1:112:B:GLU:H	2	0.22
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	10	0.22
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	7	0.22
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	17	0.22
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	8	0.22
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	13	0.22
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	4	0.22
(1,547)	1:57:B:GLU:H	1:84:B:PHE:H	17	0.22
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	14	0.22
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	9	0.22
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	15	0.22
(1,498)	1:44:B:LEU:H	1:63:B:THR:H	10	0.22
(1,498)	1:44:B:LEU:H	1:63:B:THR:H	12	0.22
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	17	0.22
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	11	0.22
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	11	0.22
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	18	0.22
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	18	0.22
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	18	0.22
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	12	0.22
(1,360)	1:122:A:THR:H	1:18:B:THR:H	10	0.22
(1,322)	1:109:A:TYR:H	1:111:A:ARG:H	17	0.22
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	1	0.22
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	10	0.22
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	10	0.22
(1,303)	1:97:A:CYS:H	1:98:A:LEU:H	16	0.22
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	8	0.22
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	4	0.22
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	4	0.22
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	4	0.22
(1,250)	1:74:A:PHE:HE1	1:126:A:LEU:HD21	4	0.22
(1,250)	1:74:A:PHE:HE1	1:126:A:LEU:HD22	4	0.22
(1,250)	1:74:A:PHE:HE1	1:126:A:LEU:HD23	4	0.22
(1,250)	1:74:A:PHE:HE2	1:126:A:LEU:HD21	4	0.22
(1,250)	1:74:A:PHE:HE2	1:126:A:LEU:HD22	4	0.22
(1,250)	1:74:A:PHE:HE2	1:126:A:LEU:HD23	4	0.22
(1,180)	1:58:A:VAL:HG11	1:59:A:VAL:H	6	0.22
(1,180)	1:58:A:VAL:HG12	1:59:A:VAL:H	6	0.22
(1,180)	1:58:A:VAL:HG13	1:59:A:VAL:H	6	0.22
(1,146)	1:50:A:GLN:H	1:57:A:GLU:H	18	0.22
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG21	15	0.22
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG22	15	0.22
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG23	15	0.22
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	15	0.22
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG21	13	0.22
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG22	13	0.22
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG23	13	0.22
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG21	13	0.22
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG22	13	0.22
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG23	13	0.22
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG21	13	0.22
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG22	13	0.22
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG23	13	0.22
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	5	0.22
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	5	0.22
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	5	0.22
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	5	0.22
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	5	0.22
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	5	0.22
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	5	0.22
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	5	0.22
(1,126)	1:44:A:LEU:HD21	1:60:A:LEU:HD11	6	0.22
(1,126)	1:44:A:LEU:HD21	1:60:A:LEU:HD12	6	0.22
(1,126)	1:44:A:LEU:HD21	1:60:A:LEU:HD13	6	0.22
(1,126)	1:44:A:LEU:HD22	1:60:A:LEU:HD11	6	0.22
(1,126)	1:44:A:LEU:HD22	1:60:A:LEU:HD12	6	0.22
(1,126)	1:44:A:LEU:HD22	1:60:A:LEU:HD13	6	0.22
(1,126)	1:44:A:LEU:HD23	1:60:A:LEU:HD11	6	0.22
(1,126)	1:44:A:LEU:HD23	1:60:A:LEU:HD12	6	0.22
(1,126)	1:44:A:LEU:HD23	1:60:A:LEU:HD13	6	0.22
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	20	0.22
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	1	0.22
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	2	0.22
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	14	0.22
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	12	0.22
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	12	0.22
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	12	0.22
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	7	0.22
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	16	0.22
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	6	0.22
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	4	0.22
(1,24)	1:17:A:TYR:H	1:81:A:GLY:H	2	0.22
(2,2)	1:40:C:VAL:O	2:290:F:TRP:NE1	8	0.21
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	13	0.21
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	13	0.21
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	13	0.21
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	13	0.21
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	13	0.21
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	13	0.21
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD11	1	0.21
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD12	1	0.21
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD13	1	0.21
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD21	1	0.21
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD22	1	0.21
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD23	1	0.21
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD11	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD12	1	0.21
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD13	1	0.21
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD21	1	0.21
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD22	1	0.21
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD23	1	0.21
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD11	1	0.21
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD12	1	0.21
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD13	1	0.21
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD21	1	0.21
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD22	1	0.21
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD23	1	0.21
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD11	1	0.21
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD12	1	0.21
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD13	1	0.21
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD21	1	0.21
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD22	1	0.21
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD23	1	0.21
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD11	1	0.21
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD12	1	0.21
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD13	1	0.21
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD21	1	0.21
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD22	1	0.21
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD23	1	0.21
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD11	1	0.21
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD12	1	0.21
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD13	1	0.21
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD21	1	0.21
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD22	1	0.21
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD23	1	0.21
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD11	9	0.21
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD12	9	0.21
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD13	9	0.21
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD11	9	0.21
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD12	9	0.21
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD13	9	0.21
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD11	9	0.21
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD12	9	0.21
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD13	9	0.21
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	10	0.21
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	10	0.21
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	10	0.21
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	10	0.21
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	10	0.21
(1,1666)	1:129:B:ALA:HB1	2:290:H:TRP:HZ3	17	0.21
(1,1666)	1:129:B:ALA:HB2	2:290:H:TRP:HZ3	17	0.21
(1,1666)	1:129:B:ALA:HB3	2:290:H:TRP:HZ3	17	0.21
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD21	12	0.21
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD22	12	0.21
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD23	12	0.21
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD21	12	0.21
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD22	12	0.21
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD23	12	0.21
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD21	12	0.21
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD22	12	0.21
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD23	12	0.21
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	1	0.21
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	1	0.21
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	1	0.21
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	1	0.21
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	1	0.21
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	1	0.21
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	5	0.21
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	5	0.21
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	5	0.21
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG21	6	0.21
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG22	6	0.21
(1,1563)	1:74:C:PHE:HZ	2:296:F:THR:HG23	6	0.21
(1,1541)	1:128:A:LEU:HD11	2:290:E:TRP:HE3	16	0.21
(1,1541)	1:128:A:LEU:HD12	2:290:E:TRP:HE3	16	0.21
(1,1541)	1:128:A:LEU:HD13	2:290:E:TRP:HE3	16	0.21
(1,1541)	1:128:A:LEU:HD21	2:290:E:TRP:HE3	16	0.21
(1,1541)	1:128:A:LEU:HD22	2:290:E:TRP:HE3	16	0.21
(1,1541)	1:128:A:LEU:HD23	2:290:E:TRP:HE3	16	0.21
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	16	0.21
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	16	0.21
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	16	0.21
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	16	0.21
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	16	0.21
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	16	0.21
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	16	0.21
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	16	0.21
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	16	0.21
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	18	0.21
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	18	0.21
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	18	0.21
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	18	0.21
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	18	0.21
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	18	0.21
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	18	0.21
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	18	0.21
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	8	0.21
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	8	0.21
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	8	0.21
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	8	0.21
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	8	0.21
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	8	0.21
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD11	6	0.21
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD12	6	0.21
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD13	6	0.21
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD21	6	0.21
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD22	6	0.21
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD23	6	0.21
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD11	6	0.21
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD12	6	0.21
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD13	6	0.21
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD21	6	0.21
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD22	6	0.21
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD23	6	0.21
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD11	6	0.21
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD12	6	0.21
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD13	6	0.21
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD21	6	0.21
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD22	6	0.21
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD23	6	0.21
(1,1514)	1:123:A:PHE:HE1	2:301:E:ILE:HD11	1	0.21
(1,1514)	1:123:A:PHE:HE1	2:301:E:ILE:HD12	1	0.21
(1,1514)	1:123:A:PHE:HE1	2:301:E:ILE:HD13	1	0.21
(1,1514)	1:123:A:PHE:HE2	2:301:E:ILE:HD11	1	0.21
(1,1514)	1:123:A:PHE:HE2	2:301:E:ILE:HD12	1	0.21
(1,1514)	1:123:A:PHE:HE2	2:301:E:ILE:HD13	1	0.21
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	13	0.21
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	13	0.21
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	13	0.21
(1,1500)	1:60:A:LEU:HD21	2:281:E:PHE:HZ	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:60:A:LEU:HD22	2:281:E:PHE:HZ	9	0.21
(1,1500)	1:60:A:LEU:HD23	2:281:E:PHE:HZ	9	0.21
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	17	0.21
(1,1462)	1:128:D:LEU:HD11	1:129:D:ALA:H	2	0.21
(1,1462)	1:128:D:LEU:HD12	1:129:D:ALA:H	2	0.21
(1,1462)	1:128:D:LEU:HD13	1:129:D:ALA:H	2	0.21
(1,1433)	1:113:D:CYS:H	1:115:D:THR:H	13	0.21
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	12	0.21
(1,1409)	1:99:D:GLY:H	1:100:D:ALA:H	15	0.21
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	17	0.21
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD11	14	0.21
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD12	14	0.21
(1,1395)	1:94:D:MET:HE1	1:98:D:LEU:HD13	14	0.21
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD11	14	0.21
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD12	14	0.21
(1,1395)	1:94:D:MET:HE2	1:98:D:LEU:HD13	14	0.21
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD11	14	0.21
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD12	14	0.21
(1,1395)	1:94:D:MET:HE3	1:98:D:LEU:HD13	14	0.21
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	17	0.21
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	5	0.21
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	17	0.21
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	9	0.21
(1,1266)	1:55:D:VAL:H	1:56:D:TYR:H	11	0.21
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	9	0.21
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	18	0.21
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	4	0.21
(1,1224)	1:42:D:LEU:HD11	1:128:D:LEU:HD11	7	0.21
(1,1224)	1:42:D:LEU:HD11	1:128:D:LEU:HD12	7	0.21
(1,1224)	1:42:D:LEU:HD11	1:128:D:LEU:HD13	7	0.21
(1,1224)	1:42:D:LEU:HD12	1:128:D:LEU:HD11	7	0.21
(1,1224)	1:42:D:LEU:HD12	1:128:D:LEU:HD12	7	0.21
(1,1224)	1:42:D:LEU:HD12	1:128:D:LEU:HD13	7	0.21
(1,1224)	1:42:D:LEU:HD13	1:128:D:LEU:HD11	7	0.21
(1,1224)	1:42:D:LEU:HD13	1:128:D:LEU:HD12	7	0.21
(1,1224)	1:42:D:LEU:HD13	1:128:D:LEU:HD13	7	0.21
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	6	0.21
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	6	0.21
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	6	0.21
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	3	0.21
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	4	0.21
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:20:D:ASP:H	1:79:D:GLN:H	10	0.21
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	7	0.21
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	3	0.21
(1,1155)	1:17:D:TYR:H	1:81:D:GLY:H	4	0.21
(1,1101)	1:126:C:LEU:HD21	1:127:C:ASN:H	14	0.21
(1,1101)	1:126:C:LEU:HD22	1:127:C:ASN:H	14	0.21
(1,1101)	1:126:C:LEU:HD23	1:127:C:ASN:H	14	0.21
(1,1039)	1:97:C:CYS:H	1:99:C:GLY:H	15	0.21
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	17	0.21
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	17	0.21
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	17	0.21
(1,922)	1:58:C:VAL:H	1:84:C:PHE:H	16	0.21
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	7	0.21
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	16	0.21
(1,909)	1:55:C:VAL:H	1:86:C:ILE:H	18	0.21
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	19	0.21
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	10	0.21
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	20	0.21
(1,849)	1:40:C:VAL:HG11	1:41:C:LYS:H	5	0.21
(1,849)	1:40:C:VAL:HG12	1:41:C:LYS:H	5	0.21
(1,849)	1:40:C:VAL:HG13	1:41:C:LYS:H	5	0.21
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	11	0.21
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	20	0.21
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	20	0.21
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	20	0.21
(1,777)	1:17:C:TYR:HE1	1:82:C:GLY:H	18	0.21
(1,777)	1:17:C:TYR:HE2	1:82:C:GLY:H	18	0.21
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	4	0.21
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	14	0.21
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	14	0.21
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	17	0.21
(1,663)	1:98:B:LEU:H	1:101:B:TYR:H	3	0.21
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	2	0.21
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	6	0.21
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	2	0.21
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	9	0.21
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	8	0.21
(1,565)	1:60:B:LEU:H	1:82:B:GLY:H	7	0.21
(1,553)	1:58:B:VAL:HG11	1:59:B:VAL:H	2	0.21
(1,553)	1:58:B:VAL:HG12	1:59:B:VAL:H	2	0.21
(1,553)	1:58:B:VAL:HG13	1:59:B:VAL:H	2	0.21
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,537)	1:55:B:VAL:H	1:56:B:TYR:HD1	8	0.21
(1,537)	1:55:B:VAL:H	1:56:B:TYR:HD2	8	0.21
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	1	0.21
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	12	0.21
(1,467)	1:33:B:GLN:H	1:35:B:ASP:H	10	0.21
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	15	0.21
(1,388)	1:136:A:LEU:H	1:138:A:MET:H	7	0.21
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	13	0.21
(1,376)	1:133:A:PHE:H	1:134:A:ASP:H	6	0.21
(1,376)	1:133:A:PHE:H	1:134:A:ASP:H	9	0.21
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	20	0.21
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	18	0.21
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	4	0.21
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	19	0.21
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	20	0.21
(1,297)	1:95:A:ALA:H	1:98:A:LEU:H	16	0.21
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	7	0.21
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	7	0.21
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	3	0.21
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	3	0.21
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	3	0.21
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	16	0.21
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	16	0.21
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	16	0.21
(1,228)	1:67:A:SER:H	1:73:A:ALA:H	3	0.21
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	18	0.21
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	18	0.21
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	4	0.21
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG11	8	0.21
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG12	8	0.21
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG13	8	0.21
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG11	8	0.21
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG12	8	0.21
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG13	8	0.21
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG11	8	0.21
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG12	8	0.21
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG13	8	0.21
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	14	0.21
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	12	0.21
(1,3)	1:10:A:THR:H	1:87:A:ALA:H	13	0.21
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	14	0.2
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	14	0.2
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	14	0.2
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	14	0.2
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	14	0.2
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	14	0.2
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	14	0.2
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	14	0.2
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	15	0.2
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	15	0.2
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	15	0.2
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	15	0.2
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	15	0.2
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	15	0.2
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	15	0.2
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	15	0.2
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	15	0.2
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD11	2	0.2
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD12	2	0.2
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD13	2	0.2
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD21	2	0.2
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD22	2	0.2
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD23	2	0.2
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD11	2	0.2
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD12	2	0.2
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD13	2	0.2
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD21	2	0.2
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD22	2	0.2
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD23	2	0.2
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD11	2	0.2
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD12	2	0.2
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD13	2	0.2
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD21	2	0.2
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD22	2	0.2
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD23	2	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	4	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	4	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	4	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	6	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	6	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	6	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	18	0.2
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	18	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	8	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	8	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	8	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	8	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	8	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	8	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	17	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	17	0.2
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	17	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	17	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	17	0.2
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	17	0.2
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	12	0.2
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	12	0.2
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	12	0.2
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	12	0.2
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	12	0.2
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	12	0.2
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	12	0.2
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	12	0.2
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	12	0.2
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	18	0.2
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	18	0.2
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	18	0.2
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	18	0.2
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	18	0.2
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	18	0.2
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	18	0.2
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	18	0.2
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	18	0.2
(1,1637)	1:98:D:LEU:HD11	2:281:G:PHE:HZ	8	0.2
(1,1637)	1:98:D:LEU:HD12	2:281:G:PHE:HZ	8	0.2
(1,1637)	1:98:D:LEU:HD13	2:281:G:PHE:HZ	8	0.2
(1,1637)	1:98:D:LEU:HD21	2:281:G:PHE:HZ	8	0.2
(1,1637)	1:98:D:LEU:HD22	2:281:G:PHE:HZ	8	0.2
(1,1637)	1:98:D:LEU:HD23	2:281:G:PHE:HZ	8	0.2
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	10	0.2
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	10	0.2
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	10	0.2
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	11	0.2
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	11	0.2
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	10	0.2
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	10	0.2
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	10	0.2
(1,1594)	1:128:C:LEU:HD11	2:290:F:TRP:HE3	5	0.2
(1,1594)	1:128:C:LEU:HD12	2:290:F:TRP:HE3	5	0.2
(1,1594)	1:128:C:LEU:HD13	2:290:F:TRP:HE3	5	0.2
(1,1594)	1:128:C:LEU:HD21	2:290:F:TRP:HE3	5	0.2
(1,1594)	1:128:C:LEU:HD22	2:290:F:TRP:HE3	5	0.2
(1,1594)	1:128:C:LEU:HD23	2:290:F:TRP:HE3	5	0.2
(1,1557)	1:106:C:LEU:HD11	2:281:F:PHE:HZ	8	0.2
(1,1557)	1:106:C:LEU:HD12	2:281:F:PHE:HZ	8	0.2
(1,1557)	1:106:C:LEU:HD13	2:281:F:PHE:HZ	8	0.2
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG21	6	0.2
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG22	6	0.2
(1,1547)	1:13:B:ILE:HD11	2:306:E:VAL:HG23	6	0.2
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG21	6	0.2
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG22	6	0.2
(1,1547)	1:13:B:ILE:HD12	2:306:E:VAL:HG23	6	0.2
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG21	6	0.2
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG22	6	0.2
(1,1547)	1:13:B:ILE:HD13	2:306:E:VAL:HG23	6	0.2
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG21	2	0.2
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG22	2	0.2
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG23	2	0.2
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG21	2	0.2
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG22	2	0.2
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG23	2	0.2
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG21	2	0.2
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG22	2	0.2
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG23	2	0.2
(1,1541)	1:128:A:LEU:HD11	2:290:E:TRP:HE3	15	0.2
(1,1541)	1:128:A:LEU:HD12	2:290:E:TRP:HE3	15	0.2
(1,1541)	1:128:A:LEU:HD13	2:290:E:TRP:HE3	15	0.2
(1,1541)	1:128:A:LEU:HD21	2:290:E:TRP:HE3	15	0.2
(1,1541)	1:128:A:LEU:HD22	2:290:E:TRP:HE3	15	0.2
(1,1541)	1:128:A:LEU:HD23	2:290:E:TRP:HE3	15	0.2
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	5	0.2
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	5	0.2
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	5	0.2
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	5	0.2
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	5	0.2
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	5	0.2
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	5	0.2
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	5	0.2
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	1	0.2
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	1	0.2
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	1	0.2
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	1	0.2
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	1	0.2
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	1	0.2
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	1	0.2
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	1	0.2
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	1	0.2
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	1	0.2
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	1	0.2
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	1	0.2
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	1	0.2
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	1	0.2
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	1	0.2
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	1	0.2
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	1	0.2
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	1	0.2
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	20	0.2
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	20	0.2
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	20	0.2
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	10	0.2
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG21	7	0.2
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG22	7	0.2
(1,1463)	1:128:D:LEU:HD11	1:131:D:VAL:HG23	7	0.2
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG21	7	0.2
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG22	7	0.2
(1,1463)	1:128:D:LEU:HD12	1:131:D:VAL:HG23	7	0.2
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG21	7	0.2
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG22	7	0.2
(1,1463)	1:128:D:LEU:HD13	1:131:D:VAL:HG23	7	0.2
(1,1462)	1:128:D:LEU:HD11	1:129:D:ALA:H	13	0.2
(1,1462)	1:128:D:LEU:HD12	1:129:D:ALA:H	13	0.2
(1,1462)	1:128:D:LEU:HD13	1:129:D:ALA:H	13	0.2
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	18	0.2
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	17	0.2
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	7	0.2
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:91:D:GLY:H	1:95:D:ALA:H	1	0.2
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	2	0.2
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	16	0.2
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	17	0.2
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	13	0.2
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	13	0.2
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	18	0.2
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	18	0.2
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	8	0.2
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	5	0.2
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	20	0.2
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	20	0.2
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	17	0.2
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	18	0.2
(1,1042)	1:98:C:LEU:H	1:99:C:GLY:H	5	0.2
(1,1042)	1:98:C:LEU:H	1:99:C:GLY:H	19	0.2
(1,1028)	1:93:C:GLN:H	1:96:C:HIS:H	16	0.2
(1,972)	1:68:C:LEU:H	1:69:C:GLY:H	8	0.2
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	1	0.2
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	7	0.2
(1,922)	1:58:C:VAL:H	1:84:C:PHE:H	15	0.2
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	1	0.2
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	17	0.2
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE1	19	0.2
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE2	19	0.2
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE1	19	0.2
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE2	19	0.2
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE1	19	0.2
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE2	19	0.2
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	3	0.2
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	16	0.2
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	2	0.2
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	11	0.2
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	7	0.2
(1,738)	1:136:B:LEU:H	1:138:B:MET:H	19	0.2
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	5	0.2
(1,706)	1:118:B:VAL:HG11	1:126:B:LEU:H	6	0.2
(1,706)	1:118:B:VAL:HG12	1:126:B:LEU:H	6	0.2
(1,706)	1:118:B:VAL:HG13	1:126:B:LEU:H	6	0.2
(1,706)	1:118:B:VAL:HG11	1:126:B:LEU:H	13	0.2
(1,706)	1:118:B:VAL:HG12	1:126:B:LEU:H	13	0.2
(1,706)	1:118:B:VAL:HG13	1:126:B:LEU:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	12	0.2
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	14	0.2
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	18	0.2
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	5	0.2
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	7	0.2
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	2	0.2
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	17	0.2
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	8	0.2
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	18	0.2
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	8	0.2
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	8	0.2
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	8	0.2
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	8	0.2
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	8	0.2
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	8	0.2
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	8	0.2
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	8	0.2
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	8	0.2
(1,644)	1:93:B:GLN:H	1:96:B:HIS:H	10	0.2
(1,640)	1:92:B:THR:H	1:94:B:MET:H	17	0.2
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	14	0.2
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB1	1	0.2
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB2	1	0.2
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB3	1	0.2
(1,546)	1:57:B:GLU:H	1:58:B:VAL:H	5	0.2
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	3	0.2
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	6	0.2
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	9	0.2
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	5	0.2
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	6	0.2
(1,421)	1:15:B:ARG:H	1:83:B:ILE:H	16	0.2
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	4	0.2
(1,413)	1:12:B:GLN:H	1:13:B:ILE:H	4	0.2
(1,396)	1:138:A:MET:H	1:141:A:LEU:H	3	0.2
(1,396)	1:138:A:MET:H	1:141:A:LEU:H	14	0.2
(1,384)	1:135:A:ALA:H	1:138:A:MET:H	11	0.2
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	3	0.2
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	13	0.2
(1,319)	1:101:A:TYR:H	1:102:A:CYS:H	14	0.2
(1,314)	1:99:A:GLY:H	1:102:A:CYS:H	16	0.2
(1,308)	1:98:A:LEU:H	1:100:A:ALA:H	9	0.2
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	15	0.2
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	18	0.2
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	12	0.2
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	12	0.2
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	12	0.2
(1,235)	1:69:A:GLY:H	1:70:A:GLU:H	17	0.2
(1,231)	1:68:A:LEU:H	1:71:A:GLU:H	7	0.2
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	10	0.2
(1,193)	1:60:A:LEU:H	1:82:A:GLY:H	16	0.2
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	4	0.2
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE1	8	0.2
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE2	8	0.2
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	16	0.2
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG21	18	0.2
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG22	18	0.2
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG23	18	0.2
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	2	0.2
(1,136)	1:47:A:ALA:H	1:59:A:VAL:H	11	0.2
(1,132)	1:45:A:ASP:H	1:63:A:THR:H	1	0.2
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	17	0.2
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	17	0.2
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	17	0.2
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	17	0.2
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	17	0.2
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	17	0.2
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	17	0.2
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	17	0.2
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	17	0.2
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	12	0.2
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	19	0.2
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	15	0.2
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	15	0.2
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	15	0.2
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	15	0.2
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	15	0.2
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	15	0.2
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	15	0.2
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	15	0.2
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	15	0.2
(1,111)	1:41:A:LYS:H	1:65:A:THR:H	3	0.2
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	1	0.2
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	19	0.2
(1,84)	1:32:A:PHE:H	1:33:A:GLN:H	13	0.2
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	20	0.2
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	20	0.2
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	9	0.2
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	9	0.2
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	11	0.2
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	11	0.2
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	2	0.2
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	12	0.2
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	16	0.19
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	16	0.19
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	16	0.19
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	16	0.19
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	16	0.19
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	16	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	3	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	3	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	3	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	3	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	3	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	3	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	13	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	13	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	13	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	13	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	13	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	13	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	20	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	20	0.19
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	20	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	20	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	20	0.19
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	20	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD11	20	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD12	20	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD13	20	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD21	20	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD22	20	0.19
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD23	20	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD11	20	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD12	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD13	20	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD21	20	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD22	20	0.19
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD23	20	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD11	20	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD12	20	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD13	20	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD21	20	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD22	20	0.19
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD23	20	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD11	20	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD12	20	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD13	20	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD21	20	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD22	20	0.19
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD23	20	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD11	20	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD12	20	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD13	20	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD21	20	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD22	20	0.19
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD23	20	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD11	20	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD12	20	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD13	20	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD21	20	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD22	20	0.19
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD23	20	0.19
(1,1630)	1:86:D:ILE:HD11	2:278:G:LEU:HD11	14	0.19
(1,1630)	1:86:D:ILE:HD11	2:278:G:LEU:HD12	14	0.19
(1,1630)	1:86:D:ILE:HD11	2:278:G:LEU:HD13	14	0.19
(1,1630)	1:86:D:ILE:HD11	2:278:G:LEU:HD21	14	0.19
(1,1630)	1:86:D:ILE:HD11	2:278:G:LEU:HD22	14	0.19
(1,1630)	1:86:D:ILE:HD11	2:278:G:LEU:HD23	14	0.19
(1,1630)	1:86:D:ILE:HD12	2:278:G:LEU:HD11	14	0.19
(1,1630)	1:86:D:ILE:HD12	2:278:G:LEU:HD12	14	0.19
(1,1630)	1:86:D:ILE:HD12	2:278:G:LEU:HD13	14	0.19
(1,1630)	1:86:D:ILE:HD12	2:278:G:LEU:HD21	14	0.19
(1,1630)	1:86:D:ILE:HD12	2:278:G:LEU:HD22	14	0.19
(1,1630)	1:86:D:ILE:HD12	2:278:G:LEU:HD23	14	0.19
(1,1630)	1:86:D:ILE:HD13	2:278:G:LEU:HD11	14	0.19
(1,1630)	1:86:D:ILE:HD13	2:278:G:LEU:HD12	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	1:86:D:ILE:HD13	2:278:G:LEU:HD13	14	0.19
(1,1630)	1:86:D:ILE:HD13	2:278:G:LEU:HD21	14	0.19
(1,1630)	1:86:D:ILE:HD13	2:278:G:LEU:HD22	14	0.19
(1,1630)	1:86:D:ILE:HD13	2:278:G:LEU:HD23	14	0.19
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD1	19	0.19
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD2	19	0.19
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD1	19	0.19
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD2	19	0.19
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD1	19	0.19
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD2	19	0.19
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG21	2	0.19
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG22	2	0.19
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG23	2	0.19
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG21	2	0.19
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG22	2	0.19
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG23	2	0.19
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG21	2	0.19
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG22	2	0.19
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG23	2	0.19
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG21	8	0.19
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG22	8	0.19
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG23	8	0.19
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG21	8	0.19
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG22	8	0.19
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG23	8	0.19
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG21	8	0.19
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG22	8	0.19
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG23	8	0.19
(1,1612)	1:58:D:VAL:HG21	2:278:G:LEU:HD11	14	0.19
(1,1612)	1:58:D:VAL:HG21	2:278:G:LEU:HD12	14	0.19
(1,1612)	1:58:D:VAL:HG21	2:278:G:LEU:HD13	14	0.19
(1,1612)	1:58:D:VAL:HG21	2:278:G:LEU:HD21	14	0.19
(1,1612)	1:58:D:VAL:HG21	2:278:G:LEU:HD22	14	0.19
(1,1612)	1:58:D:VAL:HG21	2:278:G:LEU:HD23	14	0.19
(1,1612)	1:58:D:VAL:HG22	2:278:G:LEU:HD11	14	0.19
(1,1612)	1:58:D:VAL:HG22	2:278:G:LEU:HD12	14	0.19
(1,1612)	1:58:D:VAL:HG22	2:278:G:LEU:HD13	14	0.19
(1,1612)	1:58:D:VAL:HG22	2:278:G:LEU:HD21	14	0.19
(1,1612)	1:58:D:VAL:HG22	2:278:G:LEU:HD22	14	0.19
(1,1612)	1:58:D:VAL:HG22	2:278:G:LEU:HD23	14	0.19
(1,1612)	1:58:D:VAL:HG23	2:278:G:LEU:HD11	14	0.19
(1,1612)	1:58:D:VAL:HG23	2:278:G:LEU:HD12	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1612)	1:58:D:VAL:HG23	2:278:G:LEU:HD13	14	0.19
(1,1612)	1:58:D:VAL:HG23	2:278:G:LEU:HD21	14	0.19
(1,1612)	1:58:D:VAL:HG23	2:278:G:LEU:HD22	14	0.19
(1,1612)	1:58:D:VAL:HG23	2:278:G:LEU:HD23	14	0.19
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	11	0.19
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	11	0.19
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	11	0.19
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	11	0.19
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	11	0.19
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	11	0.19
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	11	0.19
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	11	0.19
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	11	0.19
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	12	0.19
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	12	0.19
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	12	0.19
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	12	0.19
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	12	0.19
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	12	0.19
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	12	0.19
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	12	0.19
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	12	0.19
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG11	11	0.19
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG12	11	0.19
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG13	11	0.19
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG11	11	0.19
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG12	11	0.19
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG13	11	0.19
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG11	11	0.19
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG12	11	0.19
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG13	11	0.19
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD11	15	0.19
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD12	15	0.19
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD13	15	0.19
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD11	13	0.19
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD12	13	0.19
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD13	13	0.19
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD21	13	0.19
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD22	13	0.19
(1,1524)	1:86:A:ILE:HD11	2:278:E:LEU:HD23	13	0.19
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD11	13	0.19
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD12	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD13	13	0.19
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD21	13	0.19
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD22	13	0.19
(1,1524)	1:86:A:ILE:HD12	2:278:E:LEU:HD23	13	0.19
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD11	13	0.19
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD12	13	0.19
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD13	13	0.19
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD21	13	0.19
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD22	13	0.19
(1,1524)	1:86:A:ILE:HD13	2:278:E:LEU:HD23	13	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD11	12	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD12	12	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD13	12	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD21	12	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD22	12	0.19
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD23	12	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD11	12	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD12	12	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD13	12	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD21	12	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD22	12	0.19
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD23	12	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD11	12	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD12	12	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD13	12	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD21	12	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD22	12	0.19
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD23	12	0.19
(1,1516)	1:36:A:TRP:HH2	2:301:E:ILE:HD11	6	0.19
(1,1516)	1:36:A:TRP:HH2	2:301:E:ILE:HD12	6	0.19
(1,1516)	1:36:A:TRP:HH2	2:301:E:ILE:HD13	6	0.19
(1,1452)	1:118:D:VAL:HG21	1:126:D:LEU:H	9	0.19
(1,1452)	1:118:D:VAL:HG22	1:126:D:LEU:H	9	0.19
(1,1452)	1:118:D:VAL:HG23	1:126:D:LEU:H	9	0.19
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	6	0.19
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	6	0.19
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	6	0.19
(1,1449)	1:118:D:VAL:HG11	1:125:D:GLN:H	17	0.19
(1,1449)	1:118:D:VAL:HG12	1:125:D:GLN:H	17	0.19
(1,1449)	1:118:D:VAL:HG13	1:125:D:GLN:H	17	0.19
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	4	0.19
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	19	0.19
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	3	0.19
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	19	0.19
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	15	0.19
(1,1401)	1:96:D:HIS:H	1:98:D:LEU:H	13	0.19
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	9	0.19
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	4	0.19
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	12	0.19
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	16	0.19
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	16	0.19
(1,1228)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	16	0.19
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	16	0.19
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	16	0.19
(1,1228)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	16	0.19
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	16	0.19
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	16	0.19
(1,1228)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	16	0.19
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD21	11	0.19
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD22	11	0.19
(1,1211)	1:36:D:TRP:H	1:68:D:LEU:HD23	11	0.19
(1,1203)	1:33:D:GLN:H	1:35:D:ASP:H	6	0.19
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	16	0.19
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	16	0.19
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	12	0.19
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	3	0.19
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	3	0.19
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	13	0.19
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	13	0.19
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	13	0.19
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	4	0.19
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	19	0.19
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	13	0.19
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	13	0.19
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	13	0.19
(1,995)	1:77:C:GLU:H	1:78:C:VAL:H	17	0.19
(1,961)	1:66:C:ALA:H	1:73:C:ALA:H	15	0.19
(1,961)	1:66:C:ALA:H	1:73:C:ALA:H	16	0.19
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	8	0.19
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	13	0.19
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	11	0.19
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE1	4	0.19
(1,819)	1:28:C:ALA:HB1	1:17:D:TYR:HE2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE1	4	0.19
(1,819)	1:28:C:ALA:HB2	1:17:D:TYR:HE2	4	0.19
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE1	4	0.19
(1,819)	1:28:C:ALA:HB3	1:17:D:TYR:HE2	4	0.19
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	20	0.19
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	9	0.19
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	2	0.19
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	2	0.19
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	3	0.19
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	3	0.19
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	11	0.19
(1,697)	1:115:B:THR:H	1:117:B:MET:H	19	0.19
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	6	0.19
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	6	0.19
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	4	0.19
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	16	0.19
(1,664)	1:98:B:LEU:H	1:102:B:CYS:H	8	0.19
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	12	0.19
(1,644)	1:93:B:GLN:H	1:96:B:HIS:H	19	0.19
(1,640)	1:92:B:THR:H	1:94:B:MET:H	6	0.19
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	13	0.19
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	1	0.19
(1,565)	1:60:B:LEU:H	1:82:B:GLY:H	18	0.19
(1,506)	1:45:B:ASP:H	1:63:B:THR:H	7	0.19
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	3	0.19
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	3	0.19
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	3	0.19
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	3	0.19
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	11	0.19
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	11	0.19
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	11	0.19
(1,466)	1:33:B:GLN:H	1:34:B:LYS:H	12	0.19
(1,455)	1:31:B:VAL:H	1:32:B:PHE:H	3	0.19
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	6	0.19
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	10	0.19
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	14	0.19
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	12	0.19
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	5	0.19
(1,384)	1:135:A:ALA:H	1:138:A:MET:H	20	0.19
(1,381)	1:134:A:ASP:H	1:136:A:LEU:H	1	0.19
(1,368)	1:128:A:LEU:HD11	1:129:A:ALA:H	5	0.19
(1,368)	1:128:A:LEU:HD12	1:129:A:ALA:H	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:128:A:LEU:HD13	1:129:A:ALA:H	5	0.19
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	1	0.19
(1,325)	1:110:A:ALA:H	1:112:A:GLU:H	11	0.19
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	11	0.19
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	18	0.19
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	16	0.19
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	11	0.19
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	6	0.19
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	6	0.19
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	6	0.19
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	20	0.19
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	20	0.19
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	8	0.19
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	5	0.19
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	9	0.19
(1,84)	1:32:A:PHE:H	1:33:A:GLN:H	15	0.19
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	1	0.19
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	17	0.19
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	3	0.19
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	3	0.19
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	6	0.19
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	6	0.19
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	13	0.19
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	10	0.19
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	5	0.18
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	5	0.18
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	5	0.18
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	5	0.18
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	5	0.18
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	5	0.18
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	5	0.18
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	5	0.18
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	5	0.18
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG21	2	0.18
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG22	2	0.18
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG23	2	0.18
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG21	2	0.18
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG22	2	0.18
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG23	2	0.18
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG21	2	0.18
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG22	2	0.18
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG23	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	5	0.18
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	5	0.18
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	5	0.18
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	5	0.18
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	5	0.18
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	5	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD11	8	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD12	8	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD13	8	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD21	8	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD22	8	0.18
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD23	8	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD11	8	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD12	8	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD13	8	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD21	8	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD22	8	0.18
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD23	8	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD11	8	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD12	8	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD13	8	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD21	8	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD22	8	0.18
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD23	8	0.18
(1,1676)	1:94:B:MET:HE1	2:277:H:LEU:HD21	11	0.18
(1,1676)	1:94:B:MET:HE1	2:277:H:LEU:HD22	11	0.18
(1,1676)	1:94:B:MET:HE1	2:277:H:LEU:HD23	11	0.18
(1,1676)	1:94:B:MET:HE2	2:277:H:LEU:HD21	11	0.18
(1,1676)	1:94:B:MET:HE2	2:277:H:LEU:HD22	11	0.18
(1,1676)	1:94:B:MET:HE2	2:277:H:LEU:HD23	11	0.18
(1,1676)	1:94:B:MET:HE3	2:277:H:LEU:HD21	11	0.18
(1,1676)	1:94:B:MET:HE3	2:277:H:LEU:HD22	11	0.18
(1,1676)	1:94:B:MET:HE3	2:277:H:LEU:HD23	11	0.18
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	2	0.18
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	2	0.18
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	2	0.18
(1,1674)	1:32:B:PHE:HE1	2:301:H:ILE:HD11	19	0.18
(1,1674)	1:32:B:PHE:HE1	2:301:H:ILE:HD12	19	0.18
(1,1674)	1:32:B:PHE:HE1	2:301:H:ILE:HD13	19	0.18
(1,1674)	1:32:B:PHE:HE2	2:301:H:ILE:HD11	19	0.18
(1,1674)	1:32:B:PHE:HE2	2:301:H:ILE:HD12	19	0.18
(1,1674)	1:32:B:PHE:HE2	2:301:H:ILE:HD13	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1659)	1:60:B:LEU:HD21	2:281:H:PHE:HZ	13	0.18
(1,1659)	1:60:B:LEU:HD22	2:281:H:PHE:HZ	13	0.18
(1,1659)	1:60:B:LEU:HD23	2:281:H:PHE:HZ	13	0.18
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE1	3	0.18
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE2	3	0.18
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE3	3	0.18
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE1	3	0.18
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE2	3	0.18
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE3	3	0.18
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD11	5	0.18
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD12	5	0.18
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD13	5	0.18
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD11	17	0.18
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD12	17	0.18
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD13	17	0.18
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD11	17	0.18
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD12	17	0.18
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD13	17	0.18
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD11	17	0.18
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD12	17	0.18
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD13	17	0.18
(1,1637)	1:98:D:LEU:HD11	2:281:G:PHE:HZ	12	0.18
(1,1637)	1:98:D:LEU:HD12	2:281:G:PHE:HZ	12	0.18
(1,1637)	1:98:D:LEU:HD13	2:281:G:PHE:HZ	12	0.18
(1,1637)	1:98:D:LEU:HD21	2:281:G:PHE:HZ	12	0.18
(1,1637)	1:98:D:LEU:HD22	2:281:G:PHE:HZ	12	0.18
(1,1637)	1:98:D:LEU:HD23	2:281:G:PHE:HZ	12	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD11	4	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD12	4	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD13	4	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD21	4	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD22	4	0.18
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD23	4	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD11	4	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD12	4	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD13	4	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD21	4	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD22	4	0.18
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD23	4	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD11	4	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD12	4	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD13	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD21	4	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD22	4	0.18
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD23	4	0.18
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE1	14	0.18
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE2	14	0.18
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE1	14	0.18
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE2	14	0.18
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	2	0.18
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	2	0.18
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	2	0.18
(1,1603)	1:44:D:LEU:HD21	2:286:G:MET:HE1	3	0.18
(1,1603)	1:44:D:LEU:HD21	2:286:G:MET:HE2	3	0.18
(1,1603)	1:44:D:LEU:HD21	2:286:G:MET:HE3	3	0.18
(1,1603)	1:44:D:LEU:HD22	2:286:G:MET:HE1	3	0.18
(1,1603)	1:44:D:LEU:HD22	2:286:G:MET:HE2	3	0.18
(1,1603)	1:44:D:LEU:HD22	2:286:G:MET:HE3	3	0.18
(1,1603)	1:44:D:LEU:HD23	2:286:G:MET:HE1	3	0.18
(1,1603)	1:44:D:LEU:HD23	2:286:G:MET:HE2	3	0.18
(1,1603)	1:44:D:LEU:HD23	2:286:G:MET:HE3	3	0.18
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG21	2	0.18
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG22	2	0.18
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG23	2	0.18
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG21	2	0.18
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG22	2	0.18
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG23	2	0.18
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG21	2	0.18
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG22	2	0.18
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG23	2	0.18
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG21	5	0.18
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG22	5	0.18
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG23	5	0.18
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG21	5	0.18
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG22	5	0.18
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG23	5	0.18
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG21	5	0.18
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG22	5	0.18
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG23	5	0.18
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG21	19	0.18
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG22	19	0.18
(1,1598)	1:16:D:ILE:HD11	2:306:F:VAL:HG23	19	0.18
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG21	19	0.18
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG22	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	1:16:D:ILE:HD12	2:306:F:VAL:HG23	19	0.18
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG21	19	0.18
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG22	19	0.18
(1,1598)	1:16:D:ILE:HD13	2:306:F:VAL:HG23	19	0.18
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	14	0.18
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	14	0.18
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	14	0.18
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	14	0.18
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	14	0.18
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	14	0.18
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	14	0.18
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	14	0.18
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	14	0.18
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD11	6	0.18
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD12	6	0.18
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD13	6	0.18
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD11	6	0.18
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD12	6	0.18
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD13	6	0.18
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD11	6	0.18
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD12	6	0.18
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD13	6	0.18
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	8	0.18
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	8	0.18
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	8	0.18
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	8	0.18
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	8	0.18
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	8	0.18
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD11	16	0.18
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD12	16	0.18
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD13	16	0.18
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG21	14	0.18
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG22	14	0.18
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG23	14	0.18
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG21	14	0.18
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG22	14	0.18
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG23	14	0.18
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG21	14	0.18
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG22	14	0.18
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG23	14	0.18
(1,1535)	1:42:A:LEU:HD11	2:291:E:LEU:HD11	7	0.18
(1,1535)	1:42:A:LEU:HD11	2:291:E:LEU:HD12	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1535)	1:42:A:LEU:HD11	2:291:E:LEU:HD13	7	0.18
(1,1535)	1:42:A:LEU:HD12	2:291:E:LEU:HD11	7	0.18
(1,1535)	1:42:A:LEU:HD12	2:291:E:LEU:HD12	7	0.18
(1,1535)	1:42:A:LEU:HD12	2:291:E:LEU:HD13	7	0.18
(1,1535)	1:42:A:LEU:HD13	2:291:E:LEU:HD11	7	0.18
(1,1535)	1:42:A:LEU:HD13	2:291:E:LEU:HD12	7	0.18
(1,1535)	1:42:A:LEU:HD13	2:291:E:LEU:HD13	7	0.18
(1,1507)	1:129:A:ALA:HB1	2:290:E:TRP:HZ3	11	0.18
(1,1507)	1:129:A:ALA:HB2	2:290:E:TRP:HZ3	11	0.18
(1,1507)	1:129:A:ALA:HB3	2:290:E:TRP:HZ3	11	0.18
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	8	0.18
(1,1482)	1:136:D:LEU:H	1:137:D:PHE:H	15	0.18
(1,1469)	1:133:D:PHE:H	1:135:D:ALA:H	14	0.18
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	9	0.18
(1,1418)	1:101:D:TYR:H	1:102:D:CYS:H	20	0.18
(1,1376)	1:88:D:GLY:H	1:89:D:ILE:H	1	0.18
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	9	0.18
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	12	0.18
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	6	0.18
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	20	0.18
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	7	0.18
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	7	0.18
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	7	0.18
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	15	0.18
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	15	0.18
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	15	0.18
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	19	0.18
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	12	0.18
(1,1176)	1:24:D:GLU:H	1:75:D:LEU:H	17	0.18
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	12	0.18
(1,1155)	1:17:D:TYR:H	1:81:D:GLY:H	14	0.18
(1,1147)	1:14:D:GLN:H	1:15:D:ARG:H	9	0.18
(1,1130)	1:140:C:TYR:HD1	1:141:C:LEU:H	14	0.18
(1,1130)	1:140:C:TYR:HD2	1:141:C:LEU:H	14	0.18
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	11	0.18
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	7	0.18
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	10	0.18
(1,1047)	1:99:C:GLY:H	1:100:C:ALA:H	20	0.18
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	1	0.18
(1,1028)	1:93:C:GLN:H	1:96:C:HIS:H	17	0.18
(1,1011)	1:85:C:SER:H	1:86:C:ILE:H	2	0.18
(1,1007)	1:82:C:GLY:H	1:83:C:ILE:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	9	0.18
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	16	0.18
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	1	0.18
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	9	0.18
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	6	0.18
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	8	0.18
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	11	0.18
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	14	0.18
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	20	0.18
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	3	0.18
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	9	0.18
(1,821)	1:30:C:HIS:H	1:32:C:PHE:H	8	0.18
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	10	0.18
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	9	0.18
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD1	13	0.18
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD2	13	0.18
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD1	13	0.18
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD2	13	0.18
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD1	13	0.18
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD2	13	0.18
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	14	0.18
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	7	0.18
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	9	0.18
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	9	0.18
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	2	0.18
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	10	0.18
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	13	0.18
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	6	0.18
(1,577)	1:64:B:VAL:H	1:65:B:THR:H	6	0.18
(1,518)	1:51:B:LEU:H	1:55:B:VAL:H	18	0.18
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	15	0.18
(1,441)	1:23:B:PHE:H	1:24:B:GLU:H	13	0.18
(1,441)	1:23:B:PHE:H	1:24:B:GLU:H	17	0.18
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	3	0.18
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	12	0.18
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	6	0.18
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	15	0.18
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	13	0.18
(1,370)	1:128:A:LEU:HD21	1:129:A:ALA:H	5	0.18
(1,370)	1:128:A:LEU:HD22	1:129:A:ALA:H	5	0.18
(1,370)	1:128:A:LEU:HD23	1:129:A:ALA:H	5	0.18
(1,357)	1:121:A:GLY:H	1:123:A:PHE:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	10	0.18
(1,319)	1:101:A:TYR:H	1:102:A:CYS:H	10	0.18
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	13	0.18
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	10	0.18
(1,303)	1:97:A:CYS:H	1:98:A:LEU:H	19	0.18
(1,284)	1:92:A:THR:H	1:93:A:GLN:H	15	0.18
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	17	0.18
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	17	0.18
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	17	0.18
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	17	0.18
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	17	0.18
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	17	0.18
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	17	0.18
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	17	0.18
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	17	0.18
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	19	0.18
(1,146)	1:50:A:GLN:H	1:57:A:GLU:H	19	0.18
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	17	0.18
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	19	0.18
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	7	0.18
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	7	0.18
(1,125)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	7	0.18
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	7	0.18
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	7	0.18
(1,125)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	7	0.18
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	7	0.18
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	7	0.18
(1,125)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	7	0.18
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	6	0.18
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	6	0.18
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	6	0.18
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	9	0.18
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	9	0.18
(1,50)	1:23:A:PHE:H	1:21:B:ILE:H	13	0.18
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	19	0.18
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	16	0.18
(2,3)	1:40:D:VAL:O	2:290:G:TRP:NE1	20	0.17
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	7	0.17
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	7	0.17
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	7	0.17
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	7	0.17
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	7	0.17
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	7	0.17
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	7	0.17
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	7	0.17
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD11	17	0.17
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD12	17	0.17
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD13	17	0.17
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD11	17	0.17
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD12	17	0.17
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD13	17	0.17
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD11	17	0.17
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD12	17	0.17
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD13	17	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD11	15	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD12	15	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD13	15	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD21	15	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD22	15	0.17
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD23	15	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD11	15	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD12	15	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD13	15	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD21	15	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD22	15	0.17
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD23	15	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD11	15	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD12	15	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD13	15	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD21	15	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD22	15	0.17
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD23	15	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD11	15	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD12	15	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD13	15	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD21	15	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD22	15	0.17
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD23	15	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD11	15	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD12	15	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD13	15	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD21	15	0.17
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD22	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD23	15	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD11	15	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD12	15	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD13	15	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD21	15	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD22	15	0.17
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD23	15	0.17
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD11	1	0.17
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD12	1	0.17
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD13	1	0.17
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD21	1	0.17
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD22	1	0.17
(1,1681)	1:87:B:ALA:HB1	2:277:H:LEU:HD23	1	0.17
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD11	1	0.17
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD12	1	0.17
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD13	1	0.17
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD21	1	0.17
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD22	1	0.17
(1,1681)	1:87:B:ALA:HB2	2:277:H:LEU:HD23	1	0.17
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD11	1	0.17
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD12	1	0.17
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD13	1	0.17
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD21	1	0.17
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD22	1	0.17
(1,1681)	1:87:B:ALA:HB3	2:277:H:LEU:HD23	1	0.17
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	13	0.17
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	13	0.17
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	13	0.17
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	13	0.17
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	13	0.17
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	13	0.17
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	13	0.17
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	13	0.17
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	13	0.17
(1,1651)	1:129:A:ALA:HB1	2:309:G:THR:HG21	11	0.17
(1,1651)	1:129:A:ALA:HB1	2:309:G:THR:HG22	11	0.17
(1,1651)	1:129:A:ALA:HB1	2:309:G:THR:HG23	11	0.17
(1,1651)	1:129:A:ALA:HB2	2:309:G:THR:HG21	11	0.17
(1,1651)	1:129:A:ALA:HB2	2:309:G:THR:HG22	11	0.17
(1,1651)	1:129:A:ALA:HB2	2:309:G:THR:HG23	11	0.17
(1,1651)	1:129:A:ALA:HB3	2:309:G:THR:HG21	11	0.17
(1,1651)	1:129:A:ALA:HB3	2:309:G:THR:HG22	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1651)	1:129:A:ALA:HB3	2:309:G:THR:HG23	11	0.17
(1,1647)	1:128:D:LEU:HD11	2:290:G:TRP:HE3	1	0.17
(1,1647)	1:128:D:LEU:HD12	2:290:G:TRP:HE3	1	0.17
(1,1647)	1:128:D:LEU:HD13	2:290:G:TRP:HE3	1	0.17
(1,1647)	1:128:D:LEU:HD21	2:290:G:TRP:HE3	1	0.17
(1,1647)	1:128:D:LEU:HD22	2:290:G:TRP:HE3	1	0.17
(1,1647)	1:128:D:LEU:HD23	2:290:G:TRP:HE3	1	0.17
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD11	13	0.17
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD12	13	0.17
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD13	13	0.17
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD11	13	0.17
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD12	13	0.17
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD13	13	0.17
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD11	13	0.17
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD12	13	0.17
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD13	13	0.17
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	1	0.17
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	1	0.17
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	1	0.17
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	1	0.17
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	1	0.17
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	1	0.17
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	1	0.17
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	1	0.17
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	1	0.17
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD21	20	0.17
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD22	20	0.17
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD23	20	0.17
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD21	20	0.17
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD22	20	0.17
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD23	20	0.17
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD21	20	0.17
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD22	20	0.17
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD23	20	0.17
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE1	11	0.17
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE2	11	0.17
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE1	11	0.17
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE2	11	0.17
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD1	18	0.17
(1,1618)	1:68:D:LEU:HD21	2:297:G:TYR:HD2	18	0.17
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD1	18	0.17
(1,1618)	1:68:D:LEU:HD22	2:297:G:TYR:HD2	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD1	18	0.17
(1,1618)	1:68:D:LEU:HD23	2:297:G:TYR:HD2	18	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG21	17	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG22	17	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG23	17	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG21	17	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG22	17	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG23	17	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG21	17	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG22	17	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG23	17	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG21	20	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG22	20	0.17
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG23	20	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG21	20	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG22	20	0.17
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG23	20	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG21	20	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG22	20	0.17
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG23	20	0.17
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	17	0.17
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	17	0.17
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	17	0.17
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	17	0.17
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	17	0.17
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	17	0.17
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD11	15	0.17
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD12	15	0.17
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD13	15	0.17
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD21	15	0.17
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD22	15	0.17
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD23	15	0.17
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD11	15	0.17
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD12	15	0.17
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD13	15	0.17
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD21	15	0.17
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD22	15	0.17
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD23	15	0.17
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD11	15	0.17
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD12	15	0.17
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD13	15	0.17
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD21	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD22	15	0.17
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD23	15	0.17
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD11	7	0.17
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD12	7	0.17
(1,1573)	1:31:C:VAL:HG11	2:301:F:ILE:HD13	7	0.17
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD11	7	0.17
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD12	7	0.17
(1,1573)	1:31:C:VAL:HG12	2:301:F:ILE:HD13	7	0.17
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD11	7	0.17
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD12	7	0.17
(1,1573)	1:31:C:VAL:HG13	2:301:F:ILE:HD13	7	0.17
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD11	4	0.17
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD12	4	0.17
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD13	4	0.17
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD11	4	0.17
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD12	4	0.17
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD13	4	0.17
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD11	11	0.17
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD12	11	0.17
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD13	11	0.17
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD11	11	0.17
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD12	11	0.17
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD13	11	0.17
(1,1541)	1:128:A:LEU:HD11	2:290:E:TRP:HE3	18	0.17
(1,1541)	1:128:A:LEU:HD12	2:290:E:TRP:HE3	18	0.17
(1,1541)	1:128:A:LEU:HD13	2:290:E:TRP:HE3	18	0.17
(1,1541)	1:128:A:LEU:HD21	2:290:E:TRP:HE3	18	0.17
(1,1541)	1:128:A:LEU:HD22	2:290:E:TRP:HE3	18	0.17
(1,1541)	1:128:A:LEU:HD23	2:290:E:TRP:HE3	18	0.17
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	2	0.17
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	2	0.17
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	2	0.17
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	2	0.17
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	2	0.17
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	2	0.17
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD11	3	0.17
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD12	3	0.17
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD13	3	0.17
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD21	3	0.17
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD22	3	0.17
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD23	3	0.17
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD11	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD12	3	0.17
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD13	3	0.17
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD21	3	0.17
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD22	3	0.17
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD23	3	0.17
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD11	3	0.17
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD12	3	0.17
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD13	3	0.17
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD21	3	0.17
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD22	3	0.17
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD23	3	0.17
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD11	3	0.17
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD12	3	0.17
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD13	3	0.17
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD21	3	0.17
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD22	3	0.17
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD23	3	0.17
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD11	3	0.17
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD12	3	0.17
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD13	3	0.17
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD21	3	0.17
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD22	3	0.17
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD23	3	0.17
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD11	3	0.17
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD12	3	0.17
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD13	3	0.17
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD21	3	0.17
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD22	3	0.17
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD23	3	0.17
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	15	0.17
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	15	0.17
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	15	0.17
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	15	0.17
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	15	0.17
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	15	0.17
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	15	0.17
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	15	0.17
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	15	0.17
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	15	0.17
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	15	0.17
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	15	0.17
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	15	0.17
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	15	0.17
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	15	0.17
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	15	0.17
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	15	0.17
(1,1511)	1:118:A:VAL:HG11	2:296:E:THR:HG21	9	0.17
(1,1511)	1:118:A:VAL:HG11	2:296:E:THR:HG22	9	0.17
(1,1511)	1:118:A:VAL:HG11	2:296:E:THR:HG23	9	0.17
(1,1511)	1:118:A:VAL:HG12	2:296:E:THR:HG21	9	0.17
(1,1511)	1:118:A:VAL:HG12	2:296:E:THR:HG22	9	0.17
(1,1511)	1:118:A:VAL:HG12	2:296:E:THR:HG23	9	0.17
(1,1511)	1:118:A:VAL:HG13	2:296:E:THR:HG21	9	0.17
(1,1511)	1:118:A:VAL:HG13	2:296:E:THR:HG22	9	0.17
(1,1511)	1:118:A:VAL:HG13	2:296:E:THR:HG23	9	0.17
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	20	0.17
(1,1474)	1:134:D:ASP:H	1:137:D:PHE:H	3	0.17
(1,1442)	1:116:D:SER:H	1:118:D:VAL:H	12	0.17
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	1	0.17
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	15	0.17
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	16	0.17
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	18	0.17
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	8	0.17
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	13	0.17
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	15	0.17
(1,1382)	1:91:D:GLY:H	1:95:D:ALA:H	12	0.17
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB1	3	0.17
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB2	3	0.17
(1,1331)	1:68:D:LEU:HD11	1:73:D:ALA:HB3	3	0.17
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB1	3	0.17
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB2	3	0.17
(1,1331)	1:68:D:LEU:HD12	1:73:D:ALA:HB3	3	0.17
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB1	3	0.17
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB2	3	0.17
(1,1331)	1:68:D:LEU:HD13	1:73:D:ALA:HB3	3	0.17
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	2	0.17
(1,1200)	1:32:D:PHE:H	1:34:D:LYS:H	20	0.17
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	10	0.17
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	18	0.17
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	2	0.17
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	6	0.17
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	13	0.17
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	7	0.17
(1,1136)	1:10:D:THR:H	1:87:D:ALA:H	20	0.17
(1,1122)	1:136:C:LEU:H	1:139:C:ASN:H	9	0.17
(1,1122)	1:136:C:LEU:H	1:139:C:ASN:H	18	0.17
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	15	0.17
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	15	0.17
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	15	0.17
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	12	0.17
(1,1047)	1:99:C:GLY:H	1:100:C:ALA:H	4	0.17
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	5	0.17
(1,1019)	1:90:C:GLU:H	1:94:C:MET:H	10	0.17
(1,1014)	1:87:C:ALA:H	1:89:C:ILE:H	8	0.17
(1,995)	1:77:C:GLU:H	1:78:C:VAL:H	5	0.17
(1,961)	1:66:C:ALA:H	1:73:C:ALA:H	10	0.17
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	14	0.17
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	11	0.17
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	4	0.17
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	1	0.17
(1,875)	1:45:C:ASP:H	1:61:C:ARG:H	9	0.17
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	17	0.17
(1,843)	1:39:C:GLU:H	1:40:C:VAL:H	9	0.17
(1,821)	1:30:C:HIS:H	1:32:C:PHE:H	4	0.17
(1,821)	1:30:C:HIS:H	1:32:C:PHE:H	10	0.17
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	20	0.17
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	13	0.17
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	1	0.17
(1,777)	1:17:C:TYR:HE1	1:82:C:GLY:H	5	0.17
(1,777)	1:17:C:TYR:HE2	1:82:C:GLY:H	5	0.17
(1,750)	1:139:B:ASN:H	1:141:B:LEU:H	6	0.17
(1,750)	1:139:B:ASN:H	1:141:B:LEU:H	17	0.17
(1,748)	1:138:B:MET:H	1:141:B:LEU:H	5	0.17
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	12	0.17
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	7	0.17
(1,682)	1:110:B:ALA:H	1:112:B:GLU:H	3	0.17
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	11	0.17
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	2	0.17
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	20	0.17
(1,660)	1:97:B:CYS:H	1:101:B:TYR:H	20	0.17
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	3	0.17
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	16	0.17
(1,640)	1:92:B:THR:H	1:94:B:MET:H	3	0.17
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	15	0.17
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	8	0.17
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	18	0.17
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD11	3	0.17
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD12	3	0.17
(1,500)	1:44:B:LEU:HD11	1:60:B:LEU:HD13	3	0.17
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD11	3	0.17
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD12	3	0.17
(1,500)	1:44:B:LEU:HD12	1:60:B:LEU:HD13	3	0.17
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD11	3	0.17
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD12	3	0.17
(1,500)	1:44:B:LEU:HD13	1:60:B:LEU:HD13	3	0.17
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	5	0.17
(1,475)	1:36:B:TRP:HE3	1:37:B:GLN:H	13	0.17
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD21	10	0.17
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD22	10	0.17
(1,474)	1:36:B:TRP:H	1:68:B:LEU:HD23	10	0.17
(1,470)	1:35:B:ASP:H	1:36:B:TRP:HE3	15	0.17
(1,435)	1:20:B:ASP:H	1:79:B:GLN:H	18	0.17
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	20	0.17
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	18	0.17
(1,411)	1:11:B:PHE:HE1	1:12:B:GLN:H	6	0.17
(1,411)	1:11:B:PHE:HE2	1:12:B:GLN:H	6	0.17
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	16	0.17
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	16	0.17
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	3	0.17
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	15	0.17
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	6	0.17
(1,368)	1:128:A:LEU:HD11	1:129:A:ALA:H	15	0.17
(1,368)	1:128:A:LEU:HD12	1:129:A:ALA:H	15	0.17
(1,368)	1:128:A:LEU:HD13	1:129:A:ALA:H	15	0.17
(1,360)	1:122:A:THR:H	1:18:B:THR:H	13	0.17
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	2	0.17
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	8	0.17
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	14	0.17
(1,319)	1:101:A:TYR:H	1:102:A:CYS:H	9	0.17
(1,316)	1:100:A:ALA:H	1:102:A:CYS:H	11	0.17
(1,290)	1:94:A:MET:H	1:95:A:ALA:H	2	0.17
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	19	0.17
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	11	0.17
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	11	0.17
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	12	0.17
(1,208)	1:64:A:VAL:H	1:76:A:CYS:H	2	0.17
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD21	19	0.17
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD22	19	0.17
(1,184)	1:58:A:VAL:HG21	1:98:A:LEU:HD23	19	0.17
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD21	19	0.17
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD22	19	0.17
(1,184)	1:58:A:VAL:HG22	1:98:A:LEU:HD23	19	0.17
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD21	19	0.17
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD22	19	0.17
(1,184)	1:58:A:VAL:HG23	1:98:A:LEU:HD23	19	0.17
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	1	0.17
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG11	19	0.17
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG12	19	0.17
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG13	19	0.17
(1,101)	1:40:A:VAL:HG11	1:41:A:LYS:H	18	0.17
(1,101)	1:40:A:VAL:HG12	1:41:A:LYS:H	18	0.17
(1,101)	1:40:A:VAL:HG13	1:41:A:LYS:H	18	0.17
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	20	0.17
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	20	0.17
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE1	1	0.17
(1,83)	1:31:A:VAL:HG21	1:123:A:PHE:HE2	1	0.17
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE1	1	0.17
(1,83)	1:31:A:VAL:HG22	1:123:A:PHE:HE2	1	0.17
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE1	1	0.17
(1,83)	1:31:A:VAL:HG23	1:123:A:PHE:HE2	1	0.17
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	13	0.17
(1,50)	1:23:A:PHE:H	1:21:B:ILE:H	5	0.17
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	17	0.17
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	11	0.17
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	13	0.16
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	13	0.16
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	13	0.16
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	13	0.16
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	13	0.16
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	13	0.16
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	13	0.16
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	13	0.16
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	13	0.16
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG21	19	0.16
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG22	19	0.16
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG23	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG21	19	0.16
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG22	19	0.16
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG23	19	0.16
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG21	19	0.16
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG22	19	0.16
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG23	19	0.16
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD11	16	0.16
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD12	16	0.16
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD13	16	0.16
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD11	16	0.16
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD12	16	0.16
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD13	16	0.16
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD11	16	0.16
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD12	16	0.16
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD13	16	0.16
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD11	9	0.16
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD12	9	0.16
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD13	9	0.16
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD21	9	0.16
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD22	9	0.16
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD23	9	0.16
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD11	9	0.16
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD12	9	0.16
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD13	9	0.16
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD21	9	0.16
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD22	9	0.16
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD23	9	0.16
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD11	9	0.16
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD12	9	0.16
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD13	9	0.16
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD21	9	0.16
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD22	9	0.16
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD23	9	0.16
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	3	0.16
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	3	0.16
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	3	0.16
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	11	0.16
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	11	0.16
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	11	0.16
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	18	0.16
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	18	0.16
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	18	0.16
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	18	0.16
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	18	0.16
(1,1668)	1:40:B:VAL:HG11	2:290:H:TRP:HE1	14	0.16
(1,1668)	1:40:B:VAL:HG12	2:290:H:TRP:HE1	14	0.16
(1,1668)	1:40:B:VAL:HG13	2:290:H:TRP:HE1	14	0.16
(1,1663)	1:106:B:LEU:HD11	2:281:H:PHE:HZ	12	0.16
(1,1663)	1:106:B:LEU:HD12	2:281:H:PHE:HZ	12	0.16
(1,1663)	1:106:B:LEU:HD13	2:281:H:PHE:HZ	12	0.16
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG21	12	0.16
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG22	12	0.16
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG23	12	0.16
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG21	12	0.16
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG22	12	0.16
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG23	12	0.16
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD11	11	0.16
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD12	11	0.16
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD13	11	0.16
(1,1637)	1:98:D:LEU:HD11	2:281:G:PHE:HZ	17	0.16
(1,1637)	1:98:D:LEU:HD12	2:281:G:PHE:HZ	17	0.16
(1,1637)	1:98:D:LEU:HD13	2:281:G:PHE:HZ	17	0.16
(1,1637)	1:98:D:LEU:HD21	2:281:G:PHE:HZ	17	0.16
(1,1637)	1:98:D:LEU:HD22	2:281:G:PHE:HZ	17	0.16
(1,1637)	1:98:D:LEU:HD23	2:281:G:PHE:HZ	17	0.16
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	4	0.16
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	4	0.16
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	4	0.16
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	4	0.16
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	4	0.16
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	4	0.16
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	4	0.16
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	4	0.16
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	4	0.16
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD11	11	0.16
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD12	11	0.16
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD13	11	0.16
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD21	11	0.16
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD22	11	0.16
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD23	11	0.16
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD11	11	0.16
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD12	11	0.16
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD13	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD21	11	0.16
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD22	11	0.16
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD23	11	0.16
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD11	11	0.16
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD12	11	0.16
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD13	11	0.16
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD21	11	0.16
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD22	11	0.16
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD23	11	0.16
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	12	0.16
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	12	0.16
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	12	0.16
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	12	0.16
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	12	0.16
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	12	0.16
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG11	5	0.16
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG12	5	0.16
(1,1552)	1:42:C:LEU:HD21	2:288:F:VAL:HG13	5	0.16
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG11	5	0.16
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG12	5	0.16
(1,1552)	1:42:C:LEU:HD22	2:288:F:VAL:HG13	5	0.16
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG11	5	0.16
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG12	5	0.16
(1,1552)	1:42:C:LEU:HD23	2:288:F:VAL:HG13	5	0.16
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG21	16	0.16
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG22	16	0.16
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG23	16	0.16
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG21	16	0.16
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG22	16	0.16
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG23	16	0.16
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG21	16	0.16
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG22	16	0.16
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG23	16	0.16
(1,1540)	1:40:A:VAL:HG11	2:296:E:THR:HG21	18	0.16
(1,1540)	1:40:A:VAL:HG11	2:296:E:THR:HG22	18	0.16
(1,1540)	1:40:A:VAL:HG11	2:296:E:THR:HG23	18	0.16
(1,1540)	1:40:A:VAL:HG12	2:296:E:THR:HG21	18	0.16
(1,1540)	1:40:A:VAL:HG12	2:296:E:THR:HG22	18	0.16
(1,1540)	1:40:A:VAL:HG12	2:296:E:THR:HG23	18	0.16
(1,1540)	1:40:A:VAL:HG13	2:296:E:THR:HG21	18	0.16
(1,1540)	1:40:A:VAL:HG13	2:296:E:THR:HG22	18	0.16
(1,1540)	1:40:A:VAL:HG13	2:296:E:THR:HG23	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:40:A:VAL:HG21	2:296:E:THR:HG21	18	0.16
(1,1540)	1:40:A:VAL:HG21	2:296:E:THR:HG22	18	0.16
(1,1540)	1:40:A:VAL:HG21	2:296:E:THR:HG23	18	0.16
(1,1540)	1:40:A:VAL:HG22	2:296:E:THR:HG21	18	0.16
(1,1540)	1:40:A:VAL:HG22	2:296:E:THR:HG22	18	0.16
(1,1540)	1:40:A:VAL:HG22	2:296:E:THR:HG23	18	0.16
(1,1540)	1:40:A:VAL:HG23	2:296:E:THR:HG21	18	0.16
(1,1540)	1:40:A:VAL:HG23	2:296:E:THR:HG22	18	0.16
(1,1540)	1:40:A:VAL:HG23	2:296:E:THR:HG23	18	0.16
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE1	7	0.16
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE2	7	0.16
(1,1537)	1:133:A:PHE:HE1	2:286:E:MET:HE3	7	0.16
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE1	7	0.16
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE2	7	0.16
(1,1537)	1:133:A:PHE:HE2	2:286:E:MET:HE3	7	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	1	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	1	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	1	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	1	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	1	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	1	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	1	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	1	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	1	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	9	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	9	0.16
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	9	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	9	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	9	0.16
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	9	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	9	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	9	0.16
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	9	0.16
(1,1526)	1:56:A:TYR:HE1	2:277:E:LEU:HD11	13	0.16
(1,1526)	1:56:A:TYR:HE1	2:277:E:LEU:HD12	13	0.16
(1,1526)	1:56:A:TYR:HE1	2:277:E:LEU:HD13	13	0.16
(1,1526)	1:56:A:TYR:HE1	2:277:E:LEU:HD21	13	0.16
(1,1526)	1:56:A:TYR:HE1	2:277:E:LEU:HD22	13	0.16
(1,1526)	1:56:A:TYR:HE1	2:277:E:LEU:HD23	13	0.16
(1,1526)	1:56:A:TYR:HE2	2:277:E:LEU:HD11	13	0.16
(1,1526)	1:56:A:TYR:HE2	2:277:E:LEU:HD12	13	0.16
(1,1526)	1:56:A:TYR:HE2	2:277:E:LEU:HD13	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:56:A:TYR:HE2	2:277:E:LEU:HD21	13	0.16
(1,1526)	1:56:A:TYR:HE2	2:277:E:LEU:HD22	13	0.16
(1,1526)	1:56:A:TYR:HE2	2:277:E:LEU:HD23	13	0.16
(1,1509)	1:40:A:VAL:HG11	2:290:E:TRP:HE1	6	0.16
(1,1509)	1:40:A:VAL:HG12	2:290:E:TRP:HE1	6	0.16
(1,1509)	1:40:A:VAL:HG13	2:290:E:TRP:HE1	6	0.16
(1,1507)	1:129:A:ALA:HB1	2:290:E:TRP:HZ3	16	0.16
(1,1507)	1:129:A:ALA:HB2	2:290:E:TRP:HZ3	16	0.16
(1,1507)	1:129:A:ALA:HB3	2:290:E:TRP:HZ3	16	0.16
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD11	1	0.16
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD12	1	0.16
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD13	1	0.16
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD21	1	0.16
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD22	1	0.16
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD23	1	0.16
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD11	1	0.16
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD12	1	0.16
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD13	1	0.16
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD21	1	0.16
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD22	1	0.16
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD23	1	0.16
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD11	1	0.16
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD12	1	0.16
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD13	1	0.16
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD21	1	0.16
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD22	1	0.16
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD23	1	0.16
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	6	0.16
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	6	0.16
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	6	0.16
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	6	0.16
(1,1477)	1:135:D:ALA:H	1:138:D:MET:H	14	0.16
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	6	0.16
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	13	0.16
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	16	0.16
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	1	0.16
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	10	0.16
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	14	0.16
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB1	14	0.16
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB2	14	0.16
(1,1393)	1:94:D:MET:HE1	1:95:D:ALA:HB3	14	0.16
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB1	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB2	14	0.16
(1,1393)	1:94:D:MET:HE2	1:95:D:ALA:HB3	14	0.16
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB1	14	0.16
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB2	14	0.16
(1,1393)	1:94:D:MET:HE3	1:95:D:ALA:HB3	14	0.16
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	13	0.16
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	4	0.16
(1,1338)	1:73:D:ALA:H	1:74:D:PHE:H	2	0.16
(1,1330)	1:68:D:LEU:HD11	1:73:D:ALA:H	7	0.16
(1,1330)	1:68:D:LEU:HD12	1:73:D:ALA:H	7	0.16
(1,1330)	1:68:D:LEU:HD13	1:73:D:ALA:H	7	0.16
(1,1329)	1:68:D:LEU:HD11	1:71:D:GLU:H	6	0.16
(1,1329)	1:68:D:LEU:HD12	1:71:D:GLU:H	6	0.16
(1,1329)	1:68:D:LEU:HD13	1:71:D:GLU:H	6	0.16
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	11	0.16
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	9	0.16
(1,1200)	1:32:D:PHE:H	1:34:D:LYS:H	5	0.16
(1,1186)	1:30:D:HIS:H	1:32:D:PHE:H	8	0.16
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	1	0.16
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	4	0.16
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG21	12	0.16
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG22	12	0.16
(1,1181)	1:27:D:ASN:H	1:31:D:VAL:HG23	12	0.16
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	5	0.16
(1,1155)	1:17:D:TYR:H	1:81:D:GLY:H	10	0.16
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	14	0.16
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	19	0.16
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	5	0.16
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	5	0.16
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	5	0.16
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	12	0.16
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	12	0.16
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	12	0.16
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	15	0.16
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	15	0.16
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	15	0.16
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	6	0.16
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	9	0.16
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	1	0.16
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	4	0.16
(1,1050)	1:99:C:GLY:H	1:102:C:CYS:H	9	0.16
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	16	0.16
(1,1028)	1:93:C:GLN:H	1:96:C:HIS:H	20	0.16
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	12	0.16
(1,960)	1:66:C:ALA:H	1:67:C:SER:H	7	0.16
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	4	0.16
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	13	0.16
(1,909)	1:55:C:VAL:H	1:86:C:ILE:H	15	0.16
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	10	0.16
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	11	0.16
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	1	0.16
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	4	0.16
(1,876)	1:45:C:ASP:H	1:63:C:THR:H	20	0.16
(1,865)	1:43:C:ASP:H	1:44:C:LEU:H	16	0.16
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	2	0.16
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	19	0.16
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG11	2	0.16
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG12	2	0.16
(1,790)	1:20:C:ASP:H	1:59:C:VAL:HG13	2	0.16
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	19	0.16
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG11	3	0.16
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG12	3	0.16
(1,786)	1:19:C:LYS:H	1:59:C:VAL:HG13	3	0.16
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	7	0.16
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	8	0.16
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	18	0.16
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	4	0.16
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	4	0.16
(1,748)	1:138:B:MET:H	1:141:B:LEU:H	6	0.16
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	19	0.16
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	16	0.16
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	17	0.16
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	18	0.16
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	19	0.16
(1,656)	1:96:B:HIS:H	1:99:B:GLY:H	6	0.16
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	5	0.16
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	6	0.16
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	6	0.16
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	4	0.16
(1,547)	1:57:B:GLU:H	1:84:B:PHE:H	15	0.16
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	10	0.16
(1,505)	1:45:B:ASP:H	1:62:B:VAL:H	6	0.16
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	8	0.16
(1,446)	1:24:B:GLU:H	1:75:B:LEU:H	14	0.16
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	4	0.16
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	14	0.16
(1,413)	1:12:B:GLN:H	1:13:B:ILE:H	3	0.16
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD21	12	0.16
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD22	12	0.16
(1,365)	1:126:A:LEU:HD11	1:128:A:LEU:HD23	12	0.16
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD21	12	0.16
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD22	12	0.16
(1,365)	1:126:A:LEU:HD12	1:128:A:LEU:HD23	12	0.16
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD21	12	0.16
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD22	12	0.16
(1,365)	1:126:A:LEU:HD13	1:128:A:LEU:HD23	12	0.16
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	3	0.16
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	4	0.16
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	6	0.16
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	13	0.16
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	16	0.16
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	15	0.16
(1,302)	1:96:A:HIS:H	1:99:A:GLY:H	20	0.16
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD11	15	0.16
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD12	15	0.16
(1,294)	1:94:A:MET:HE1	1:98:A:LEU:HD13	15	0.16
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD11	15	0.16
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD12	15	0.16
(1,294)	1:94:A:MET:HE2	1:98:A:LEU:HD13	15	0.16
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD11	15	0.16
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD12	15	0.16
(1,294)	1:94:A:MET:HE3	1:98:A:LEU:HD13	15	0.16
(1,284)	1:92:A:THR:H	1:93:A:GLN:H	10	0.16
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	2	0.16
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	20	0.16
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	10	0.16
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	10	0.16
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	10	0.16
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB1	20	0.16
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB2	20	0.16
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB3	20	0.16
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB1	20	0.16
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB2	20	0.16
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB3	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB1	20	0.16
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB2	20	0.16
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB3	20	0.16
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	8	0.16
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	20	0.16
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE1	19	0.16
(1,167)	1:55:A:VAL:H	1:56:A:TYR:HE2	19	0.16
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG21	19	0.16
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG22	19	0.16
(1,144)	1:49:A:SER:H	1:58:A:VAL:HG23	19	0.16
(1,131)	1:45:A:ASP:H	1:62:A:VAL:H	9	0.16
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	11	0.16
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG11	2	0.16
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG12	2	0.16
(1,110)	1:41:A:LYS:H	1:64:A:VAL:HG13	2	0.16
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD11	10	0.16
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD12	10	0.16
(1,103)	1:40:A:VAL:HG11	1:126:A:LEU:HD13	10	0.16
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD11	10	0.16
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD12	10	0.16
(1,103)	1:40:A:VAL:HG12	1:126:A:LEU:HD13	10	0.16
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD11	10	0.16
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD12	10	0.16
(1,103)	1:40:A:VAL:HG13	1:126:A:LEU:HD13	10	0.16
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG11	2	0.16
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG12	2	0.16
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG13	2	0.16
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG11	2	0.16
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG12	2	0.16
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG13	2	0.16
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG11	2	0.16
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG12	2	0.16
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG13	2	0.16
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	8	0.16
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	8	0.16
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	8	0.16
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	12	0.16
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	16	0.16
(1,62)	1:28:A:ALA:H	1:30:A:HIS:H	15	0.16
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	12	0.16
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	19	0.16
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:40:A:VAL:O	2:290:E:TRP:NE1	4	0.15
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD11	5	0.15
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD12	5	0.15
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD13	5	0.15
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD21	5	0.15
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD22	5	0.15
(1,1688)	1:98:B:LEU:HD11	2:280:H:LEU:HD23	5	0.15
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD11	5	0.15
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD12	5	0.15
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD13	5	0.15
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD21	5	0.15
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD22	5	0.15
(1,1688)	1:98:B:LEU:HD12	2:280:H:LEU:HD23	5	0.15
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD11	5	0.15
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD12	5	0.15
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD13	5	0.15
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD21	5	0.15
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD22	5	0.15
(1,1688)	1:98:B:LEU:HD13	2:280:H:LEU:HD23	5	0.15
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD11	5	0.15
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD12	5	0.15
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD13	5	0.15
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD21	5	0.15
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD22	5	0.15
(1,1688)	1:98:B:LEU:HD21	2:280:H:LEU:HD23	5	0.15
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD11	5	0.15
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD12	5	0.15
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD13	5	0.15
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD21	5	0.15
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD22	5	0.15
(1,1688)	1:98:B:LEU:HD22	2:280:H:LEU:HD23	5	0.15
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD11	5	0.15
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD12	5	0.15
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD13	5	0.15
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD21	5	0.15
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD22	5	0.15
(1,1688)	1:98:B:LEU:HD23	2:280:H:LEU:HD23	5	0.15
(1,1685)	1:56:B:TYR:HE1	2:277:H:LEU:HD11	3	0.15
(1,1685)	1:56:B:TYR:HE1	2:277:H:LEU:HD12	3	0.15
(1,1685)	1:56:B:TYR:HE1	2:277:H:LEU:HD13	3	0.15
(1,1685)	1:56:B:TYR:HE1	2:277:H:LEU:HD21	3	0.15
(1,1685)	1:56:B:TYR:HE1	2:277:H:LEU:HD22	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:56:B:TYR:HE1	2:277:H:LEU:HD23	3	0.15
(1,1685)	1:56:B:TYR:HE2	2:277:H:LEU:HD11	3	0.15
(1,1685)	1:56:B:TYR:HE2	2:277:H:LEU:HD12	3	0.15
(1,1685)	1:56:B:TYR:HE2	2:277:H:LEU:HD13	3	0.15
(1,1685)	1:56:B:TYR:HE2	2:277:H:LEU:HD21	3	0.15
(1,1685)	1:56:B:TYR:HE2	2:277:H:LEU:HD22	3	0.15
(1,1685)	1:56:B:TYR:HE2	2:277:H:LEU:HD23	3	0.15
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	6	0.15
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	6	0.15
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	6	0.15
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	6	0.15
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	6	0.15
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	6	0.15
(1,1666)	1:129:B:ALA:HB1	2:290:H:TRP:HZ3	11	0.15
(1,1666)	1:129:B:ALA:HB2	2:290:H:TRP:HZ3	11	0.15
(1,1666)	1:129:B:ALA:HB3	2:290:H:TRP:HZ3	11	0.15
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD11	20	0.15
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD12	20	0.15
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD13	20	0.15
(1,1659)	1:60:B:LEU:HD21	2:281:H:PHE:HZ	3	0.15
(1,1659)	1:60:B:LEU:HD22	2:281:H:PHE:HZ	3	0.15
(1,1659)	1:60:B:LEU:HD23	2:281:H:PHE:HZ	3	0.15
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE1	20	0.15
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE2	20	0.15
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE3	20	0.15
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE1	20	0.15
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE2	20	0.15
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE3	20	0.15
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	17	0.15
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	17	0.15
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	17	0.15
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	17	0.15
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	17	0.15
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	17	0.15
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	17	0.15
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	17	0.15
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	17	0.15
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD11	7	0.15
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD12	7	0.15
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD13	7	0.15
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD11	1	0.15
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD12	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD13	1	0.15
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD11	1	0.15
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD12	1	0.15
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD13	1	0.15
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD11	1	0.15
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD12	1	0.15
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD13	1	0.15
(1,1637)	1:98:D:LEU:HD11	2:281:G:PHE:HZ	13	0.15
(1,1637)	1:98:D:LEU:HD12	2:281:G:PHE:HZ	13	0.15
(1,1637)	1:98:D:LEU:HD13	2:281:G:PHE:HZ	13	0.15
(1,1637)	1:98:D:LEU:HD21	2:281:G:PHE:HZ	13	0.15
(1,1637)	1:98:D:LEU:HD22	2:281:G:PHE:HZ	13	0.15
(1,1637)	1:98:D:LEU:HD23	2:281:G:PHE:HZ	13	0.15
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD11	10	0.15
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD12	10	0.15
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD13	10	0.15
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD21	10	0.15
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD22	10	0.15
(1,1628)	1:87:D:ALA:HB1	2:277:G:LEU:HD23	10	0.15
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD11	10	0.15
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD12	10	0.15
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD13	10	0.15
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD21	10	0.15
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD22	10	0.15
(1,1628)	1:87:D:ALA:HB2	2:277:G:LEU:HD23	10	0.15
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD11	10	0.15
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD12	10	0.15
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD13	10	0.15
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD21	10	0.15
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD22	10	0.15
(1,1628)	1:87:D:ALA:HB3	2:277:G:LEU:HD23	10	0.15
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE1	3	0.15
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE2	3	0.15
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE1	3	0.15
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE2	3	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD11	5	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD12	5	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD13	5	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD21	5	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD22	5	0.15
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD23	5	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD11	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD12	5	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD13	5	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD21	5	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD22	5	0.15
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD23	5	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD11	5	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD12	5	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD13	5	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD21	5	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD22	5	0.15
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD23	5	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD11	5	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD12	5	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD13	5	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD21	5	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD22	5	0.15
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD23	5	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD11	5	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD12	5	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD13	5	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD21	5	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD22	5	0.15
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD23	5	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD11	5	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD12	5	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD13	5	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD21	5	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD22	5	0.15
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD23	5	0.15
(1,1569)	1:36:C:TRP:HH2	2:301:F:ILE:HD11	6	0.15
(1,1569)	1:36:C:TRP:HH2	2:301:F:ILE:HD12	6	0.15
(1,1569)	1:36:C:TRP:HH2	2:301:F:ILE:HD13	6	0.15
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE1	6	0.15
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE2	6	0.15
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE1	6	0.15
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE2	6	0.15
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	13	0.15
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	13	0.15
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	13	0.15
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	13	0.15
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	13	0.15
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1562)	1:40:C:VAL:HG11	2:290:F:TRP:HE1	5	0.15
(1,1562)	1:40:C:VAL:HG12	2:290:F:TRP:HE1	5	0.15
(1,1562)	1:40:C:VAL:HG13	2:290:F:TRP:HE1	5	0.15
(1,1562)	1:40:C:VAL:HG11	2:290:F:TRP:HE1	8	0.15
(1,1562)	1:40:C:VAL:HG12	2:290:F:TRP:HE1	8	0.15
(1,1562)	1:40:C:VAL:HG13	2:290:F:TRP:HE1	8	0.15
(1,1556)	1:56:C:TYR:HE1	2:278:F:LEU:HD21	11	0.15
(1,1556)	1:56:C:TYR:HE1	2:278:F:LEU:HD22	11	0.15
(1,1556)	1:56:C:TYR:HE1	2:278:F:LEU:HD23	11	0.15
(1,1556)	1:56:C:TYR:HE2	2:278:F:LEU:HD21	11	0.15
(1,1556)	1:56:C:TYR:HE2	2:278:F:LEU:HD22	11	0.15
(1,1556)	1:56:C:TYR:HE2	2:278:F:LEU:HD23	11	0.15
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	20	0.15
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	20	0.15
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	20	0.15
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	20	0.15
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	20	0.15
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	20	0.15
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	20	0.15
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	20	0.15
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	20	0.15
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	15	0.15
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	15	0.15
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	15	0.15
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	15	0.15
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	15	0.15
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	15	0.15
(1,1530)	1:98:A:LEU:HD11	2:281:E:PHE:HD1	18	0.15
(1,1530)	1:98:A:LEU:HD11	2:281:E:PHE:HD2	18	0.15
(1,1530)	1:98:A:LEU:HD12	2:281:E:PHE:HD1	18	0.15
(1,1530)	1:98:A:LEU:HD12	2:281:E:PHE:HD2	18	0.15
(1,1530)	1:98:A:LEU:HD13	2:281:E:PHE:HD1	18	0.15
(1,1530)	1:98:A:LEU:HD13	2:281:E:PHE:HD2	18	0.15
(1,1530)	1:98:A:LEU:HD21	2:281:E:PHE:HD1	18	0.15
(1,1530)	1:98:A:LEU:HD21	2:281:E:PHE:HD2	18	0.15
(1,1530)	1:98:A:LEU:HD22	2:281:E:PHE:HD1	18	0.15
(1,1530)	1:98:A:LEU:HD22	2:281:E:PHE:HD2	18	0.15
(1,1530)	1:98:A:LEU:HD23	2:281:E:PHE:HD1	18	0.15
(1,1530)	1:98:A:LEU:HD23	2:281:E:PHE:HD2	18	0.15
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD11	2	0.15
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD12	2	0.15
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD13	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD21	2	0.15
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD22	2	0.15
(1,1525)	1:94:A:MET:HE1	2:278:E:LEU:HD23	2	0.15
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD11	2	0.15
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD12	2	0.15
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD13	2	0.15
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD21	2	0.15
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD22	2	0.15
(1,1525)	1:94:A:MET:HE2	2:278:E:LEU:HD23	2	0.15
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD11	2	0.15
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD12	2	0.15
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD13	2	0.15
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD21	2	0.15
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD22	2	0.15
(1,1525)	1:94:A:MET:HE3	2:278:E:LEU:HD23	2	0.15
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	15	0.15
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	15	0.15
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	15	0.15
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	3	0.15
(1,1459)	1:126:D:LEU:HD21	1:128:D:LEU:H	16	0.15
(1,1459)	1:126:D:LEU:HD22	1:128:D:LEU:H	16	0.15
(1,1459)	1:126:D:LEU:HD23	1:128:D:LEU:H	16	0.15
(1,1442)	1:116:D:SER:H	1:118:D:VAL:H	17	0.15
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	5	0.15
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	8	0.15
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	20	0.15
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	3	0.15
(1,1407)	1:98:D:LEU:H	1:100:D:ALA:H	5	0.15
(1,1405)	1:97:D:CYS:H	1:100:D:ALA:H	14	0.15
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	15	0.15
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	20	0.15
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	12	0.15
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	14	0.15
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	16	0.15
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	19	0.15
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	6	0.15
(1,1338)	1:73:D:ALA:H	1:74:D:PHE:H	18	0.15
(1,1290)	1:60:D:LEU:H	1:82:D:GLY:H	16	0.15
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	2	0.15
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	3	0.15
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	8	0.15
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	15	0.15
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	18	0.15
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB1	1	0.15
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB2	1	0.15
(1,1214)	1:39:D:GLU:H	1:66:D:ALA:HB3	1	0.15
(1,1190)	1:31:D:VAL:HG11	1:34:D:LYS:H	9	0.15
(1,1190)	1:31:D:VAL:HG12	1:34:D:LYS:H	9	0.15
(1,1190)	1:31:D:VAL:HG13	1:34:D:LYS:H	9	0.15
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	2	0.15
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	9	0.15
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	12	0.15
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB1	13	0.15
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB2	13	0.15
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB3	13	0.15
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB1	13	0.15
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB2	13	0.15
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB3	13	0.15
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB1	13	0.15
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB2	13	0.15
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB3	13	0.15
(1,1174)	1:23:D:PHE:HE1	1:75:D:LEU:H	4	0.15
(1,1174)	1:23:D:PHE:HE2	1:75:D:LEU:H	4	0.15
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	1	0.15
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	14	0.15
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	7	0.15
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	7	0.15
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	8	0.15
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	3	0.15
(1,1047)	1:99:C:GLY:H	1:100:C:ALA:H	12	0.15
(1,1047)	1:99:C:GLY:H	1:100:C:ALA:H	19	0.15
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	5	0.15
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	5	0.15
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	5	0.15
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	14	0.15
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	14	0.15
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	14	0.15
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	15	0.15
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	15	0.15
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	15	0.15
(1,995)	1:77:C:GLU:H	1:78:C:VAL:H	14	0.15
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	4	0.15
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	4	0.15
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	4	0.15
(1,961)	1:66:C:ALA:H	1:73:C:ALA:H	8	0.15
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	13	0.15
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	14	0.15
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	9	0.15
(1,913)	1:56:C:TYR:H	1:85:C:SER:H	10	0.15
(1,913)	1:56:C:TYR:H	1:85:C:SER:H	16	0.15
(1,909)	1:55:C:VAL:H	1:86:C:ILE:H	1	0.15
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	6	0.15
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	5	0.15
(1,876)	1:45:C:ASP:H	1:63:C:THR:H	17	0.15
(1,841)	1:36:C:TRP:HE3	1:37:C:GLN:H	5	0.15
(1,840)	1:36:C:TRP:H	1:37:C:GLN:H	9	0.15
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	2	0.15
(1,792)	1:20:C:ASP:H	1:81:C:GLY:H	16	0.15
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	14	0.15
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	6	0.15
(1,782)	1:18:C:THR:H	1:81:C:GLY:H	1	0.15
(1,768)	1:14:C:GLN:H	1:85:C:SER:H	1	0.15
(1,765)	1:14:C:GLN:H	1:15:C:ARG:H	6	0.15
(1,748)	1:138:B:MET:H	1:141:B:LEU:H	2	0.15
(1,722)	1:128:B:LEU:HD21	1:129:B:ALA:H	10	0.15
(1,722)	1:128:B:LEU:HD22	1:129:B:ALA:H	10	0.15
(1,722)	1:128:B:LEU:HD23	1:129:B:ALA:H	10	0.15
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	6	0.15
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	6	0.15
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	6	0.15
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	16	0.15
(1,698)	1:116:B:SER:H	1:117:B:MET:H	14	0.15
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	6	0.15
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	10	0.15
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	15	0.15
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD1	3	0.15
(1,674)	1:100:B:ALA:HB1	1:133:B:PHE:HD2	3	0.15
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD1	3	0.15
(1,674)	1:100:B:ALA:HB2	1:133:B:PHE:HD2	3	0.15
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD1	3	0.15
(1,674)	1:100:B:ALA:HB3	1:133:B:PHE:HD2	3	0.15
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	1	0.15
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	11	0.15
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	16	0.15
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	12	0.15
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB1	19	0.15
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB2	19	0.15
(1,598)	1:68:B:LEU:HD11	1:73:B:ALA:HB3	19	0.15
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB1	19	0.15
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB2	19	0.15
(1,598)	1:68:B:LEU:HD12	1:73:B:ALA:HB3	19	0.15
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB1	19	0.15
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB2	19	0.15
(1,598)	1:68:B:LEU:HD13	1:73:B:ALA:HB3	19	0.15
(1,553)	1:58:B:VAL:HG11	1:59:B:VAL:H	9	0.15
(1,553)	1:58:B:VAL:HG12	1:59:B:VAL:H	9	0.15
(1,553)	1:58:B:VAL:HG13	1:59:B:VAL:H	9	0.15
(1,521)	1:51:B:LEU:H	1:57:B:GLU:H	6	0.15
(1,506)	1:45:B:ASP:H	1:63:B:THR:H	5	0.15
(1,498)	1:44:B:LEU:H	1:63:B:THR:H	2	0.15
(1,496)	1:43:B:ASP:H	1:65:B:THR:H	5	0.15
(1,491)	1:42:B:LEU:HD21	1:43:B:ASP:H	14	0.15
(1,491)	1:42:B:LEU:HD22	1:43:B:ASP:H	14	0.15
(1,491)	1:42:B:LEU:HD23	1:43:B:ASP:H	14	0.15
(1,479)	1:39:B:GLU:H	1:68:B:LEU:H	3	0.15
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD21	19	0.15
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD22	19	0.15
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD23	19	0.15
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	2	0.15
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	2	0.15
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	2	0.15
(1,468)	1:34:B:LYS:H	1:35:B:ASP:H	11	0.15
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	11	0.15
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	11	0.15
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	11	0.15
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	11	0.15
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	11	0.15
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	11	0.15
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	11	0.15
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	11	0.15
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	11	0.15
(1,397)	1:138:A:MET:HE1	1:141:A:LEU:HD21	8	0.15
(1,397)	1:138:A:MET:HE1	1:141:A:LEU:HD22	8	0.15
(1,397)	1:138:A:MET:HE1	1:141:A:LEU:HD23	8	0.15
(1,397)	1:138:A:MET:HE2	1:141:A:LEU:HD21	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:138:A:MET:HE2	1:141:A:LEU:HD22	8	0.15
(1,397)	1:138:A:MET:HE2	1:141:A:LEU:HD23	8	0.15
(1,397)	1:138:A:MET:HE3	1:141:A:LEU:HD21	8	0.15
(1,397)	1:138:A:MET:HE3	1:141:A:LEU:HD22	8	0.15
(1,397)	1:138:A:MET:HE3	1:141:A:LEU:HD23	8	0.15
(1,396)	1:138:A:MET:H	1:141:A:LEU:H	7	0.15
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	12	0.15
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	12	0.15
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	12	0.15
(1,376)	1:133:A:PHE:H	1:134:A:ASP:H	1	0.15
(1,376)	1:133:A:PHE:H	1:134:A:ASP:H	18	0.15
(1,360)	1:122:A:THR:H	1:18:B:THR:H	7	0.15
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	1	0.15
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	12	0.15
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	14	0.15
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	20	0.15
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	4	0.15
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	12	0.15
(1,319)	1:101:A:TYR:H	1:102:A:CYS:H	1	0.15
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	2	0.15
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	5	0.15
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	3	0.15
(1,302)	1:96:A:HIS:H	1:99:A:GLY:H	8	0.15
(1,292)	1:94:A:MET:H	1:97:A:CYS:H	12	0.15
(1,285)	1:92:A:THR:H	1:94:A:MET:H	1	0.15
(1,285)	1:92:A:THR:H	1:94:A:MET:H	7	0.15
(1,277)	1:88:A:GLY:H	1:89:A:ILE:H	6	0.15
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	5	0.15
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	8	0.15
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	13	0.15
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	5	0.15
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	5	0.15
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	5	0.15
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	5	0.15
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	5	0.15
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	5	0.15
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	5	0.15
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	5	0.15
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	5	0.15
(1,205)	1:63:A:THR:H	1:78:A:VAL:H	8	0.15
(1,198)	1:62:A:VAL:H	1:63:A:THR:H	16	0.15
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:51:A:LEU:H	1:55:A:VAL:H	9	0.15
(1,146)	1:50:A:GLN:H	1:57:A:GLU:H	14	0.15
(1,136)	1:47:A:ALA:H	1:59:A:VAL:H	8	0.15
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG21	5	0.15
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG22	5	0.15
(1,128)	1:44:A:LEU:HD21	1:62:A:VAL:HG23	5	0.15
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG21	5	0.15
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG22	5	0.15
(1,128)	1:44:A:LEU:HD22	1:62:A:VAL:HG23	5	0.15
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG21	5	0.15
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG22	5	0.15
(1,128)	1:44:A:LEU:HD23	1:62:A:VAL:HG23	5	0.15
(1,122)	1:44:A:LEU:H	1:63:A:THR:H	16	0.15
(1,111)	1:41:A:LYS:H	1:65:A:THR:H	10	0.15
(1,111)	1:41:A:LYS:H	1:65:A:THR:H	12	0.15
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	1	0.15
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	9	0.15
(1,85)	1:32:A:PHE:H	1:34:A:LYS:H	17	0.15
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	13	0.15
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	9	0.15
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	14	0.15
(1,50)	1:23:A:PHE:H	1:21:B:ILE:H	16	0.15
(1,44)	1:21:A:ILE:H	1:25:B:ALA:H	13	0.15
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	19	0.15
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	20	0.15
(1,24)	1:17:A:TYR:H	1:81:A:GLY:H	7	0.15
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	9	0.15
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	4	0.15
(2,2)	1:40:C:VAL:O	2:290:F:TRP:NE1	10	0.14
(2,2)	1:40:C:VAL:O	2:290:F:TRP:NE1	16	0.14
(1,1700)	1:128:B:LEU:HD11	2:290:H:TRP:HE3	2	0.14
(1,1700)	1:128:B:LEU:HD12	2:290:H:TRP:HE3	2	0.14
(1,1700)	1:128:B:LEU:HD13	2:290:H:TRP:HE3	2	0.14
(1,1700)	1:128:B:LEU:HD21	2:290:H:TRP:HE3	2	0.14
(1,1700)	1:128:B:LEU:HD22	2:290:H:TRP:HE3	2	0.14
(1,1700)	1:128:B:LEU:HD23	2:290:H:TRP:HE3	2	0.14
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD11	7	0.14
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD12	7	0.14
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD13	7	0.14
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD11	7	0.14
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD12	7	0.14
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD13	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD11	7	0.14
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD12	7	0.14
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD13	7	0.14
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	1	0.14
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	1	0.14
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	1	0.14
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	1	0.14
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	1	0.14
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	1	0.14
(1,1659)	1:60:B:LEU:HD21	2:281:H:PHE:HZ	4	0.14
(1,1659)	1:60:B:LEU:HD22	2:281:H:PHE:HZ	4	0.14
(1,1659)	1:60:B:LEU:HD23	2:281:H:PHE:HZ	4	0.14
(1,1658)	1:42:B:LEU:HD21	2:288:H:VAL:HG11	20	0.14
(1,1658)	1:42:B:LEU:HD21	2:288:H:VAL:HG12	20	0.14
(1,1658)	1:42:B:LEU:HD21	2:288:H:VAL:HG13	20	0.14
(1,1658)	1:42:B:LEU:HD22	2:288:H:VAL:HG11	20	0.14
(1,1658)	1:42:B:LEU:HD22	2:288:H:VAL:HG12	20	0.14
(1,1658)	1:42:B:LEU:HD22	2:288:H:VAL:HG13	20	0.14
(1,1658)	1:42:B:LEU:HD23	2:288:H:VAL:HG11	20	0.14
(1,1658)	1:42:B:LEU:HD23	2:288:H:VAL:HG12	20	0.14
(1,1658)	1:42:B:LEU:HD23	2:288:H:VAL:HG13	20	0.14
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	1	0.14
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	1	0.14
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	1	0.14
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	1	0.14
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	1	0.14
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	1	0.14
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	1	0.14
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	1	0.14
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	1	0.14
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	5	0.14
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	5	0.14
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	5	0.14
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	5	0.14
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	5	0.14
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	5	0.14
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	5	0.14
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	5	0.14
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	5	0.14
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD11	6	0.14
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD12	6	0.14
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD13	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD11	5	0.14
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD12	5	0.14
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD13	5	0.14
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD21	5	0.14
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD22	5	0.14
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD23	5	0.14
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD11	5	0.14
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD12	5	0.14
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD13	5	0.14
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD21	5	0.14
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD22	5	0.14
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD23	5	0.14
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD11	5	0.14
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD12	5	0.14
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD13	5	0.14
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD21	5	0.14
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD22	5	0.14
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD23	5	0.14
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	7	0.14
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	7	0.14
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	7	0.14
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	7	0.14
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	7	0.14
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	7	0.14
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	7	0.14
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	7	0.14
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	7	0.14
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD21	13	0.14
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD22	13	0.14
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD23	13	0.14
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD21	13	0.14
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD22	13	0.14
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD23	13	0.14
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD21	13	0.14
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD22	13	0.14
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD23	13	0.14
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD11	9	0.14
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD12	9	0.14
(1,1622)	1:36:D:TRP:HH2	2:301:G:ILE:HD13	9	0.14
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD11	11	0.14
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD12	11	0.14
(1,1621)	1:32:D:PHE:HE1	2:301:G:ILE:HD13	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD11	11	0.14
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD12	11	0.14
(1,1621)	1:32:D:PHE:HE2	2:301:G:ILE:HD13	11	0.14
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE1	13	0.14
(1,1619)	1:123:D:PHE:HE1	2:297:G:TYR:HE2	13	0.14
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE1	13	0.14
(1,1619)	1:123:D:PHE:HE2	2:297:G:TYR:HE2	13	0.14
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG21	11	0.14
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG22	11	0.14
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG23	11	0.14
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	7	0.14
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	7	0.14
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	7	0.14
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	11	0.14
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	11	0.14
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	11	0.14
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	14	0.14
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	14	0.14
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	14	0.14
(1,1610)	1:106:D:LEU:HD11	2:281:G:PHE:HZ	3	0.14
(1,1610)	1:106:D:LEU:HD12	2:281:G:PHE:HZ	3	0.14
(1,1610)	1:106:D:LEU:HD13	2:281:G:PHE:HZ	3	0.14
(1,1594)	1:128:C:LEU:HD11	2:290:F:TRP:HE3	1	0.14
(1,1594)	1:128:C:LEU:HD12	2:290:F:TRP:HE3	1	0.14
(1,1594)	1:128:C:LEU:HD13	2:290:F:TRP:HE3	1	0.14
(1,1594)	1:128:C:LEU:HD21	2:290:F:TRP:HE3	1	0.14
(1,1594)	1:128:C:LEU:HD22	2:290:F:TRP:HE3	1	0.14
(1,1594)	1:128:C:LEU:HD23	2:290:F:TRP:HE3	1	0.14
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD11	13	0.14
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD12	13	0.14
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD13	13	0.14
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD21	13	0.14
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD22	13	0.14
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD23	13	0.14
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD11	13	0.14
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD12	13	0.14
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD13	13	0.14
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD21	13	0.14
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD22	13	0.14
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD23	13	0.14
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD11	13	0.14
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD12	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD13	13	0.14
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD21	13	0.14
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD22	13	0.14
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD23	13	0.14
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD11	13	0.14
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD12	13	0.14
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD13	13	0.14
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD21	13	0.14
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD22	13	0.14
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD23	13	0.14
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD11	13	0.14
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD12	13	0.14
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD13	13	0.14
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD21	13	0.14
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD22	13	0.14
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD23	13	0.14
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD11	13	0.14
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD12	13	0.14
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD13	13	0.14
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD21	13	0.14
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD22	13	0.14
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD23	13	0.14
(1,1578)	1:94:C:MET:HE1	2:278:F:LEU:HD11	2	0.14
(1,1578)	1:94:C:MET:HE1	2:278:F:LEU:HD12	2	0.14
(1,1578)	1:94:C:MET:HE1	2:278:F:LEU:HD13	2	0.14
(1,1578)	1:94:C:MET:HE1	2:278:F:LEU:HD21	2	0.14
(1,1578)	1:94:C:MET:HE1	2:278:F:LEU:HD22	2	0.14
(1,1578)	1:94:C:MET:HE1	2:278:F:LEU:HD23	2	0.14
(1,1578)	1:94:C:MET:HE2	2:278:F:LEU:HD11	2	0.14
(1,1578)	1:94:C:MET:HE2	2:278:F:LEU:HD12	2	0.14
(1,1578)	1:94:C:MET:HE2	2:278:F:LEU:HD13	2	0.14
(1,1578)	1:94:C:MET:HE2	2:278:F:LEU:HD21	2	0.14
(1,1578)	1:94:C:MET:HE2	2:278:F:LEU:HD22	2	0.14
(1,1578)	1:94:C:MET:HE2	2:278:F:LEU:HD23	2	0.14
(1,1578)	1:94:C:MET:HE3	2:278:F:LEU:HD11	2	0.14
(1,1578)	1:94:C:MET:HE3	2:278:F:LEU:HD12	2	0.14
(1,1578)	1:94:C:MET:HE3	2:278:F:LEU:HD13	2	0.14
(1,1578)	1:94:C:MET:HE3	2:278:F:LEU:HD21	2	0.14
(1,1578)	1:94:C:MET:HE3	2:278:F:LEU:HD22	2	0.14
(1,1578)	1:94:C:MET:HE3	2:278:F:LEU:HD23	2	0.14
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE1	8	0.14
(1,1566)	1:123:C:PHE:HE1	2:297:F:TYR:HE2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE1	8	0.14
(1,1566)	1:123:C:PHE:HE2	2:297:F:TYR:HE2	8	0.14
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	7	0.14
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	7	0.14
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	7	0.14
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	7	0.14
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	7	0.14
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	7	0.14
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG21	8	0.14
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG22	8	0.14
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG23	8	0.14
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG21	8	0.14
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG22	8	0.14
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG23	8	0.14
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG21	8	0.14
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG22	8	0.14
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG23	8	0.14
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG21	17	0.14
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG22	17	0.14
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG23	17	0.14
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG21	17	0.14
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG22	17	0.14
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG23	17	0.14
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG21	17	0.14
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG22	17	0.14
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG23	17	0.14
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD11	6	0.14
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD12	6	0.14
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD13	6	0.14
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	11	0.14
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	11	0.14
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	11	0.14
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	11	0.14
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	11	0.14
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	11	0.14
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	11	0.14
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	11	0.14
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	11	0.14
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	5	0.14
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	5	0.14
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	5	0.14
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	5	0.14
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	5	0.14
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD11	17	0.14
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD12	17	0.14
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD13	17	0.14
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD21	17	0.14
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD22	17	0.14
(1,1523)	1:89:A:ILE:HD11	2:277:E:LEU:HD23	17	0.14
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD11	17	0.14
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD12	17	0.14
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD13	17	0.14
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD21	17	0.14
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD22	17	0.14
(1,1523)	1:89:A:ILE:HD12	2:277:E:LEU:HD23	17	0.14
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD11	17	0.14
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD12	17	0.14
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD13	17	0.14
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD21	17	0.14
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD22	17	0.14
(1,1523)	1:89:A:ILE:HD13	2:277:E:LEU:HD23	17	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	13	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	13	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	13	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	13	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	13	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	13	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	13	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	13	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	13	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	13	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	13	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	13	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	13	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	13	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	13	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	13	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	13	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	13	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	20	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	20	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	20	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	20	0.14
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	20	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	20	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	20	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	20	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	20	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	20	0.14
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	20	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	20	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	20	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	20	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	20	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	20	0.14
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	20	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD11	5	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD12	5	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD13	5	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD11	5	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD12	5	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD13	5	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD11	5	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD12	5	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD13	5	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD11	7	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD12	7	0.14
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD13	7	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD11	7	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD12	7	0.14
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD13	7	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD11	7	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD12	7	0.14
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD13	7	0.14
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD11	4	0.14
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD12	4	0.14
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD13	4	0.14
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD21	4	0.14
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD22	4	0.14
(1,1506)	1:58:A:VAL:HG21	2:278:E:LEU:HD23	4	0.14
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD11	4	0.14
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD12	4	0.14
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD13	4	0.14
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD21	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD22	4	0.14
(1,1506)	1:58:A:VAL:HG22	2:278:E:LEU:HD23	4	0.14
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD11	4	0.14
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD12	4	0.14
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD13	4	0.14
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD21	4	0.14
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD22	4	0.14
(1,1506)	1:58:A:VAL:HG23	2:278:E:LEU:HD23	4	0.14
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	7	0.14
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	7	0.14
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	7	0.14
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	16	0.14
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	16	0.14
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	16	0.14
(1,1485)	1:137:D:PHE:H	1:139:D:ASN:H	1	0.14
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	2	0.14
(1,1483)	1:136:D:LEU:H	1:138:D:MET:H	4	0.14
(1,1469)	1:133:D:PHE:H	1:135:D:ALA:H	4	0.14
(1,1433)	1:113:D:CYS:H	1:115:D:THR:H	6	0.14
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	2	0.14
(1,1405)	1:97:D:CYS:H	1:100:D:ALA:H	15	0.14
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	5	0.14
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	14	0.14
(1,1382)	1:91:D:GLY:H	1:95:D:ALA:H	14	0.14
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	4	0.14
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	6	0.14
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	11	0.14
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	13	0.14
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	6	0.14
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	20	0.14
(1,1304)	1:64:D:VAL:H	1:65:D:THR:H	3	0.14
(1,1268)	1:55:D:VAL:H	1:56:D:TYR:HE1	17	0.14
(1,1268)	1:55:D:VAL:H	1:56:D:TYR:HE2	17	0.14
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	20	0.14
(1,1229)	1:43:D:ASP:H	1:44:D:LEU:H	3	0.14
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	13	0.14
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	9	0.14
(1,1147)	1:14:D:GLN:H	1:15:D:ARG:H	19	0.14
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	9	0.14
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	9	0.14
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	9	0.14
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	19	0.14
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	19	0.14
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	4	0.14
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	4	0.14
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	4	0.14
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	19	0.14
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	19	0.14
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	19	0.14
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	12	0.14
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	11	0.14
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	18	0.14
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	5	0.14
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	19	0.14
(1,1033)	1:95:C:ALA:H	1:98:C:LEU:H	2	0.14
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	10	0.14
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	18	0.14
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	20	0.14
(1,1007)	1:82:C:GLY:H	1:83:C:ILE:H	1	0.14
(1,1007)	1:82:C:GLY:H	1:83:C:ILE:H	6	0.14
(1,1007)	1:82:C:GLY:H	1:83:C:ILE:H	15	0.14
(1,995)	1:77:C:GLU:H	1:78:C:VAL:H	13	0.14
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	6	0.14
(1,989)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	6	0.14
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	6	0.14
(1,989)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	6	0.14
(1,960)	1:66:C:ALA:H	1:67:C:SER:H	3	0.14
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	1	0.14
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	20	0.14
(1,914)	1:56:C:TYR:H	1:86:C:ILE:H	18	0.14
(1,909)	1:55:C:VAL:H	1:86:C:ILE:H	3	0.14
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	8	0.14
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	10	0.14
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	18	0.14
(1,875)	1:45:C:ASP:H	1:61:C:ARG:H	16	0.14
(1,845)	1:39:C:GLU:H	1:67:C:SER:H	10	0.14
(1,843)	1:39:C:GLU:H	1:40:C:VAL:H	2	0.14
(1,816)	1:28:C:ALA:H	1:30:C:HIS:H	9	0.14
(1,798)	1:22:C:SER:H	1:78:C:VAL:H	2	0.14
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	10	0.14
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	10	0.14
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	10	0.14
(1,757)	1:11:C:PHE:HD1	1:12:C:GLN:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,757)	1:11:C:PHE:HD2	1:12:C:GLN:H	14	0.14
(1,738)	1:136:B:LEU:H	1:138:B:MET:H	9	0.14
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	6	0.14
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	18	0.14
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD1	6	0.14
(1,710)	1:118:B:VAL:HG21	1:123:B:PHE:HD2	6	0.14
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD1	6	0.14
(1,710)	1:118:B:VAL:HG22	1:123:B:PHE:HD2	6	0.14
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD1	6	0.14
(1,710)	1:118:B:VAL:HG23	1:123:B:PHE:HD2	6	0.14
(1,696)	1:115:B:THR:H	1:116:B:SER:H	1	0.14
(1,696)	1:115:B:THR:H	1:116:B:SER:H	17	0.14
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	6	0.14
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	20	0.14
(1,669)	1:99:B:GLY:H	1:102:B:CYS:H	11	0.14
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	16	0.14
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	3	0.14
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	19	0.14
(1,657)	1:97:B:CYS:H	1:98:B:LEU:H	17	0.14
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	9	0.14
(1,630)	1:87:B:ALA:H	1:89:B:ILE:H	17	0.14
(1,595)	1:68:B:LEU:H	1:73:B:ALA:H	3	0.14
(1,594)	1:68:B:LEU:H	1:71:B:GLU:H	5	0.14
(1,547)	1:57:B:GLU:H	1:84:B:PHE:H	6	0.14
(1,546)	1:57:B:GLU:H	1:58:B:VAL:H	2	0.14
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	20	0.14
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	3	0.14
(1,452)	1:28:B:ALA:H	1:31:B:VAL:H	17	0.14
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	1	0.14
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	2	0.14
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	1	0.14
(1,413)	1:12:B:GLN:H	1:13:B:ILE:H	7	0.14
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	20	0.14
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	20	0.14
(1,383)	1:135:A:ALA:H	1:137:A:PHE:H	2	0.14
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	5	0.14
(1,360)	1:122:A:THR:H	1:18:B:THR:H	18	0.14
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	9	0.14
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	15	0.14
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	7	0.14
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	9	0.14
(1,321)	1:109:A:TYR:H	1:110:A:ALA:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	15	0.14
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	16	0.14
(1,303)	1:97:A:CYS:H	1:98:A:LEU:H	6	0.14
(1,302)	1:96:A:HIS:H	1:99:A:GLY:H	17	0.14
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	1	0.14
(1,293)	1:94:A:MET:HE1	1:95:A:ALA:H	12	0.14
(1,293)	1:94:A:MET:HE2	1:95:A:ALA:H	12	0.14
(1,293)	1:94:A:MET:HE3	1:95:A:ALA:H	12	0.14
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	12	0.14
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	7	0.14
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	15	0.14
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB1	5	0.14
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB2	5	0.14
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB3	5	0.14
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB1	5	0.14
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB2	5	0.14
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB3	5	0.14
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB1	5	0.14
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB2	5	0.14
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB3	5	0.14
(1,228)	1:67:A:SER:H	1:73:A:ALA:H	15	0.14
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	5	0.14
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG21	19	0.14
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG22	19	0.14
(1,195)	1:60:A:LEU:HD11	1:62:A:VAL:HG23	19	0.14
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG21	19	0.14
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG22	19	0.14
(1,195)	1:60:A:LEU:HD12	1:62:A:VAL:HG23	19	0.14
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG21	19	0.14
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG22	19	0.14
(1,195)	1:60:A:LEU:HD13	1:62:A:VAL:HG23	19	0.14
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	7	0.14
(1,151)	1:51:A:LEU:H	1:57:A:GLU:H	20	0.14
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG11	10	0.14
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG12	10	0.14
(1,135)	1:47:A:ALA:H	1:58:A:VAL:HG13	10	0.14
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG11	6	0.14
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG12	6	0.14
(1,127)	1:44:A:LEU:HD21	1:62:A:VAL:HG13	6	0.14
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG11	6	0.14
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG12	6	0.14
(1,127)	1:44:A:LEU:HD22	1:62:A:VAL:HG13	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG11	6	0.14
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG12	6	0.14
(1,127)	1:44:A:LEU:HD23	1:62:A:VAL:HG13	6	0.14
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	3	0.14
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD21	20	0.14
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD22	20	0.14
(1,117)	1:42:A:LEU:HD21	1:44:A:LEU:HD23	20	0.14
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD21	20	0.14
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD22	20	0.14
(1,117)	1:42:A:LEU:HD22	1:44:A:LEU:HD23	20	0.14
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD21	20	0.14
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD22	20	0.14
(1,117)	1:42:A:LEU:HD23	1:44:A:LEU:HD23	20	0.14
(1,99)	1:39:A:GLU:H	1:67:A:SER:H	17	0.14
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB1	4	0.14
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB2	4	0.14
(1,98)	1:39:A:GLU:H	1:66:A:ALA:HB3	4	0.14
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	17	0.14
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	17	0.14
(1,70)	1:30:A:HIS:H	1:33:A:GLN:H	4	0.14
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	3	0.14
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	4	0.14
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	10	0.14
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	20	0.14
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	10	0.14
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	17	0.14
(1,3)	1:10:A:THR:H	1:87:A:ALA:H	19	0.14
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	7	0.13
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	4	0.13
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	4	0.13
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	4	0.13
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	4	0.13
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	4	0.13
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	4	0.13
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	4	0.13
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	4	0.13
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	4	0.13
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG21	8	0.13
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG22	8	0.13
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG23	8	0.13
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG21	8	0.13
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG22	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG23	8	0.13
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG21	8	0.13
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG22	8	0.13
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG23	8	0.13
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG21	9	0.13
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG22	9	0.13
(1,1704)	1:16:A:ILE:HD11	2:306:H:VAL:HG23	9	0.13
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG21	9	0.13
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG22	9	0.13
(1,1704)	1:16:A:ILE:HD12	2:306:H:VAL:HG23	9	0.13
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG21	9	0.13
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG22	9	0.13
(1,1704)	1:16:A:ILE:HD13	2:306:H:VAL:HG23	9	0.13
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD11	9	0.13
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD12	9	0.13
(1,1691)	1:128:B:LEU:HD11	2:291:H:LEU:HD13	9	0.13
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD11	9	0.13
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD12	9	0.13
(1,1691)	1:128:B:LEU:HD12	2:291:H:LEU:HD13	9	0.13
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD11	9	0.13
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD12	9	0.13
(1,1691)	1:128:B:LEU:HD13	2:291:H:LEU:HD13	9	0.13
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD11	7	0.13
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD12	7	0.13
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD13	7	0.13
(1,1662)	1:56:B:TYR:HE1	2:278:H:LEU:HD21	9	0.13
(1,1662)	1:56:B:TYR:HE1	2:278:H:LEU:HD22	9	0.13
(1,1662)	1:56:B:TYR:HE1	2:278:H:LEU:HD23	9	0.13
(1,1662)	1:56:B:TYR:HE2	2:278:H:LEU:HD21	9	0.13
(1,1662)	1:56:B:TYR:HE2	2:278:H:LEU:HD22	9	0.13
(1,1662)	1:56:B:TYR:HE2	2:278:H:LEU:HD23	9	0.13
(1,1659)	1:60:B:LEU:HD21	2:281:H:PHE:HZ	11	0.13
(1,1659)	1:60:B:LEU:HD22	2:281:H:PHE:HZ	11	0.13
(1,1659)	1:60:B:LEU:HD23	2:281:H:PHE:HZ	11	0.13
(1,1647)	1:128:D:LEU:HD11	2:290:G:TRP:HE3	12	0.13
(1,1647)	1:128:D:LEU:HD12	2:290:G:TRP:HE3	12	0.13
(1,1647)	1:128:D:LEU:HD13	2:290:G:TRP:HE3	12	0.13
(1,1647)	1:128:D:LEU:HD21	2:290:G:TRP:HE3	12	0.13
(1,1647)	1:128:D:LEU:HD22	2:290:G:TRP:HE3	12	0.13
(1,1647)	1:128:D:LEU:HD23	2:290:G:TRP:HE3	12	0.13
(1,1644)	1:136:D:LEU:HD11	2:286:G:MET:HE1	20	0.13
(1,1644)	1:136:D:LEU:HD11	2:286:G:MET:HE2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:136:D:LEU:HD11	2:286:G:MET:HE3	20	0.13
(1,1644)	1:136:D:LEU:HD12	2:286:G:MET:HE1	20	0.13
(1,1644)	1:136:D:LEU:HD12	2:286:G:MET:HE2	20	0.13
(1,1644)	1:136:D:LEU:HD12	2:286:G:MET:HE3	20	0.13
(1,1644)	1:136:D:LEU:HD13	2:286:G:MET:HE1	20	0.13
(1,1644)	1:136:D:LEU:HD13	2:286:G:MET:HE2	20	0.13
(1,1644)	1:136:D:LEU:HD13	2:286:G:MET:HE3	20	0.13
(1,1644)	1:136:D:LEU:HD21	2:286:G:MET:HE1	20	0.13
(1,1644)	1:136:D:LEU:HD21	2:286:G:MET:HE2	20	0.13
(1,1644)	1:136:D:LEU:HD21	2:286:G:MET:HE3	20	0.13
(1,1644)	1:136:D:LEU:HD22	2:286:G:MET:HE1	20	0.13
(1,1644)	1:136:D:LEU:HD22	2:286:G:MET:HE2	20	0.13
(1,1644)	1:136:D:LEU:HD22	2:286:G:MET:HE3	20	0.13
(1,1644)	1:136:D:LEU:HD23	2:286:G:MET:HE1	20	0.13
(1,1644)	1:136:D:LEU:HD23	2:286:G:MET:HE2	20	0.13
(1,1644)	1:136:D:LEU:HD23	2:286:G:MET:HE3	20	0.13
(1,1642)	1:129:D:ALA:HB1	2:291:G:LEU:HD21	11	0.13
(1,1642)	1:129:D:ALA:HB1	2:291:G:LEU:HD22	11	0.13
(1,1642)	1:129:D:ALA:HB1	2:291:G:LEU:HD23	11	0.13
(1,1642)	1:129:D:ALA:HB2	2:291:G:LEU:HD21	11	0.13
(1,1642)	1:129:D:ALA:HB2	2:291:G:LEU:HD22	11	0.13
(1,1642)	1:129:D:ALA:HB2	2:291:G:LEU:HD23	11	0.13
(1,1642)	1:129:D:ALA:HB3	2:291:G:LEU:HD21	11	0.13
(1,1642)	1:129:D:ALA:HB3	2:291:G:LEU:HD22	11	0.13
(1,1642)	1:129:D:ALA:HB3	2:291:G:LEU:HD23	11	0.13
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD11	12	0.13
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD12	12	0.13
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD13	12	0.13
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD11	12	0.13
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD12	12	0.13
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD13	12	0.13
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD11	12	0.13
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD12	12	0.13
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD13	12	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD11	14	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD12	14	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD13	14	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD21	14	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD22	14	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD23	14	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD11	14	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD12	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD13	14	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD21	14	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD22	14	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD23	14	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD11	14	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD12	14	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD13	14	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD21	14	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD22	14	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD23	14	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD11	14	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD12	14	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD13	14	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD21	14	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD22	14	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD23	14	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD11	14	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD12	14	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD13	14	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD21	14	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD22	14	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD23	14	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD11	14	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD12	14	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD13	14	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD21	14	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD22	14	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD23	14	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD11	15	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD12	15	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD13	15	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD21	15	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD22	15	0.13
(1,1635)	1:98:D:LEU:HD11	2:280:G:LEU:HD23	15	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD11	15	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD12	15	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD13	15	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD21	15	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD22	15	0.13
(1,1635)	1:98:D:LEU:HD12	2:280:G:LEU:HD23	15	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD11	15	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD12	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD13	15	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD21	15	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD22	15	0.13
(1,1635)	1:98:D:LEU:HD13	2:280:G:LEU:HD23	15	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD11	15	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD12	15	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD13	15	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD21	15	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD22	15	0.13
(1,1635)	1:98:D:LEU:HD21	2:280:G:LEU:HD23	15	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD11	15	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD12	15	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD13	15	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD21	15	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD22	15	0.13
(1,1635)	1:98:D:LEU:HD22	2:280:G:LEU:HD23	15	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD11	15	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD12	15	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD13	15	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD21	15	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD22	15	0.13
(1,1635)	1:98:D:LEU:HD23	2:280:G:LEU:HD23	15	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD11	3	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD12	3	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD13	3	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD21	3	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD22	3	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD23	3	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD11	3	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD12	3	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD13	3	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD21	3	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD22	3	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD23	3	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD11	3	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD12	3	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD13	3	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD21	3	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD22	3	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD23	3	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD11	16	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD12	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD13	16	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD21	16	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD22	16	0.13
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD23	16	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD11	16	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD12	16	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD13	16	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD21	16	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD22	16	0.13
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD23	16	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD11	16	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD12	16	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD13	16	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD21	16	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD22	16	0.13
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD23	16	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD11	19	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD12	19	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD13	19	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD21	19	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD22	19	0.13
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD23	19	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD11	19	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD12	19	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD13	19	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD21	19	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD22	19	0.13
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD23	19	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD11	19	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD12	19	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD13	19	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD21	19	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD22	19	0.13
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD23	19	0.13
(1,1624)	1:129:D:ALA:HB1	2:288:G:VAL:HG11	6	0.13
(1,1624)	1:129:D:ALA:HB1	2:288:G:VAL:HG12	6	0.13
(1,1624)	1:129:D:ALA:HB1	2:288:G:VAL:HG13	6	0.13
(1,1624)	1:129:D:ALA:HB2	2:288:G:VAL:HG11	6	0.13
(1,1624)	1:129:D:ALA:HB2	2:288:G:VAL:HG12	6	0.13
(1,1624)	1:129:D:ALA:HB2	2:288:G:VAL:HG13	6	0.13
(1,1624)	1:129:D:ALA:HB3	2:288:G:VAL:HG11	6	0.13
(1,1624)	1:129:D:ALA:HB3	2:288:G:VAL:HG12	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1624)	1:129:D:ALA:HB3	2:288:G:VAL:HG13	6	0.13
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD21	17	0.13
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD22	17	0.13
(1,1623)	1:94:D:MET:HE1	2:277:G:LEU:HD23	17	0.13
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD21	17	0.13
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD22	17	0.13
(1,1623)	1:94:D:MET:HE2	2:277:G:LEU:HD23	17	0.13
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD21	17	0.13
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD22	17	0.13
(1,1623)	1:94:D:MET:HE3	2:277:G:LEU:HD23	17	0.13
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG21	13	0.13
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG22	13	0.13
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG23	13	0.13
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG21	13	0.13
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG22	13	0.13
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG23	13	0.13
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG21	13	0.13
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG22	13	0.13
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG23	13	0.13
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	2	0.13
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	2	0.13
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	2	0.13
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	2	0.13
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	2	0.13
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	2	0.13
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	2	0.13
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	2	0.13
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	2	0.13
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD11	8	0.13
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD12	8	0.13
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD13	8	0.13
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD11	8	0.13
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD12	8	0.13
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD13	8	0.13
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD11	15	0.13
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD12	15	0.13
(1,1558)	1:137:C:PHE:HZ	2:280:F:LEU:HD13	15	0.13
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG21	1	0.13
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG22	1	0.13
(1,1546)	1:131:D:VAL:HG21	2:309:E:THR:HG23	1	0.13
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG21	1	0.13
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG22	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:131:D:VAL:HG22	2:309:E:THR:HG23	1	0.13
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG21	1	0.13
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG22	1	0.13
(1,1546)	1:131:D:VAL:HG23	2:309:E:THR:HG23	1	0.13
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD11	18	0.13
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD12	18	0.13
(1,1543)	1:36:A:TRP:HE3	2:301:E:ILE:HD13	18	0.13
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	15	0.13
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	15	0.13
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	15	0.13
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	15	0.13
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	15	0.13
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	15	0.13
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	15	0.13
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	15	0.13
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	15	0.13
(1,1531)	1:98:A:LEU:HD11	2:281:E:PHE:HZ	7	0.13
(1,1531)	1:98:A:LEU:HD12	2:281:E:PHE:HZ	7	0.13
(1,1531)	1:98:A:LEU:HD13	2:281:E:PHE:HZ	7	0.13
(1,1531)	1:98:A:LEU:HD21	2:281:E:PHE:HZ	7	0.13
(1,1531)	1:98:A:LEU:HD22	2:281:E:PHE:HZ	7	0.13
(1,1531)	1:98:A:LEU:HD23	2:281:E:PHE:HZ	7	0.13
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD11	4	0.13
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD12	4	0.13
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD13	4	0.13
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD21	4	0.13
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD22	4	0.13
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD23	4	0.13
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD11	4	0.13
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD12	4	0.13
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD13	4	0.13
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD21	4	0.13
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD22	4	0.13
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD23	4	0.13
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD11	4	0.13
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD12	4	0.13
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD13	4	0.13
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD21	4	0.13
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD22	4	0.13
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD23	4	0.13
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD11	4	0.13
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD12	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD13	4	0.13
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD21	4	0.13
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD22	4	0.13
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD23	4	0.13
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD11	4	0.13
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD12	4	0.13
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD13	4	0.13
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD21	4	0.13
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD22	4	0.13
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD23	4	0.13
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD11	4	0.13
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD12	4	0.13
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD13	4	0.13
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD21	4	0.13
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD22	4	0.13
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD23	4	0.13
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	7	0.13
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	7	0.13
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	7	0.13
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	7	0.13
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	7	0.13
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	7	0.13
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	7	0.13
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	7	0.13
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	7	0.13
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	7	0.13
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	7	0.13
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	7	0.13
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	7	0.13
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	7	0.13
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	7	0.13
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	7	0.13
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	7	0.13
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	7	0.13
(1,1482)	1:136:D:LEU:H	1:137:D:PHE:H	8	0.13
(1,1436)	1:114:D:ILE:H	1:116:D:SER:H	19	0.13
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	2	0.13
(1,1433)	1:113:D:CYS:H	1:115:D:THR:H	5	0.13
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	4	0.13
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	13	0.13
(1,1409)	1:99:D:GLY:H	1:100:D:ALA:H	19	0.13
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	3	0.13
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	7	0.13
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	1	0.13
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD21	19	0.13
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD22	19	0.13
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD23	19	0.13
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	5	0.13
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	7	0.13
(1,1326)	1:68:D:LEU:H	1:71:D:GLU:H	11	0.13
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	9	0.13
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	12	0.13
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	12	0.13
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	12	0.13
(1,1310)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	12	0.13
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	12	0.13
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	12	0.13
(1,1310)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	12	0.13
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	12	0.13
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	12	0.13
(1,1310)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	12	0.13
(1,1251)	1:51:D:LEU:H	1:52:D:ALA:H	6	0.13
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	5	0.13
(1,1246)	1:49:D:SER:H	1:50:D:GLN:H	18	0.13
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD11	18	0.13
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD12	18	0.13
(1,1236)	1:45:D:ASP:H	1:60:D:LEU:HD13	18	0.13
(1,1200)	1:32:D:PHE:H	1:34:D:LYS:H	9	0.13
(1,1182)	1:28:D:ALA:H	1:30:D:HIS:H	10	0.13
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	5	0.13
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	19	0.13
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	9	0.13
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	10	0.13
(1,1159)	1:19:D:LYS:H	1:20:D:ASP:H	14	0.13
(1,1145)	1:12:D:GLN:H	1:85:D:SER:H	11	0.13
(1,1140)	1:11:D:PHE:HD1	1:12:D:GLN:H	5	0.13
(1,1140)	1:11:D:PHE:HD2	1:12:D:GLN:H	5	0.13
(1,1131)	1:140:C:TYR:HE1	1:141:C:LEU:H	11	0.13
(1,1131)	1:140:C:TYR:HE2	1:141:C:LEU:H	11	0.13
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	4	0.13
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	4	0.13
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	4	0.13
(1,1107)	1:128:C:LEU:HD21	1:129:C:ALA:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:128:C:LEU:HD22	1:129:C:ALA:H	11	0.13
(1,1107)	1:128:C:LEU:HD23	1:129:C:ALA:H	11	0.13
(1,1095)	1:122:C:THR:H	1:18:D:THR:H	9	0.13
(1,1095)	1:122:C:THR:H	1:18:D:THR:H	17	0.13
(1,1092)	1:121:C:GLY:H	1:123:C:PHE:H	14	0.13
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	14	0.13
(1,1050)	1:99:C:GLY:H	1:102:C:CYS:H	20	0.13
(1,1038)	1:97:C:CYS:H	1:98:C:LEU:H	6	0.13
(1,1038)	1:97:C:CYS:H	1:98:C:LEU:H	18	0.13
(1,1033)	1:95:C:ALA:H	1:98:C:LEU:H	3	0.13
(1,1016)	1:88:C:GLY:H	1:89:C:ILE:H	20	0.13
(1,995)	1:77:C:GLU:H	1:78:C:VAL:H	18	0.13
(1,961)	1:66:C:ALA:H	1:73:C:ALA:H	14	0.13
(1,913)	1:56:C:TYR:H	1:85:C:SER:H	3	0.13
(1,913)	1:56:C:TYR:H	1:85:C:SER:H	9	0.13
(1,890)	1:51:C:LEU:H	1:55:C:VAL:H	6	0.13
(1,888)	1:50:C:GLN:H	1:57:C:GLU:H	9	0.13
(1,886)	1:49:C:SER:H	1:57:C:GLU:H	19	0.13
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB1	12	0.13
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB2	12	0.13
(1,844)	1:39:C:GLU:H	1:66:C:ALA:HB3	12	0.13
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD21	17	0.13
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD22	17	0.13
(1,839)	1:35:C:ASP:H	1:68:C:LEU:HD23	17	0.13
(1,829)	1:31:C:VAL:HG21	1:36:C:TRP:HZ3	3	0.13
(1,829)	1:31:C:VAL:HG22	1:36:C:TRP:HZ3	3	0.13
(1,829)	1:31:C:VAL:HG23	1:36:C:TRP:HZ3	3	0.13
(1,801)	1:23:C:PHE:H	1:24:C:GLU:H	1	0.13
(1,787)	1:19:C:LYS:H	1:79:C:GLN:H	6	0.13
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	17	0.13
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB1	16	0.13
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB2	16	0.13
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB3	16	0.13
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB1	16	0.13
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB2	16	0.13
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB3	16	0.13
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	2	0.13
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	2	0.13
(1,731)	1:134:B:ASP:H	1:135:B:ALA:H	4	0.13
(1,692)	1:113:B:CYS:H	1:116:B:SER:H	14	0.13
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	8	0.13
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	17	0.13
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	18	0.13
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	12	0.13
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	11	0.13
(1,651)	1:95:B:ALA:H	1:98:B:LEU:H	17	0.13
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	18	0.13
(1,627)	1:85:B:SER:H	1:86:B:ILE:H	20	0.13
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	5	0.13
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	5	0.13
(1,557)	1:59:B:VAL:H	1:60:B:LEU:H	13	0.13
(1,543)	1:56:B:TYR:H	1:86:B:ILE:H	11	0.13
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	3	0.13
(1,501)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	3	0.13
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	3	0.13
(1,501)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	3	0.13
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	3	0.13
(1,501)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	3	0.13
(1,475)	1:36:B:TRP:HE3	1:37:B:GLN:H	12	0.13
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	8	0.13
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	8	0.13
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	8	0.13
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	8	0.13
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	8	0.13
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	8	0.13
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	8	0.13
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	8	0.13
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	8	0.13
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	13	0.13
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	6	0.13
(1,376)	1:133:A:PHE:H	1:134:A:ASP:H	12	0.13
(1,357)	1:121:A:GLY:H	1:123:A:PHE:H	1	0.13
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	10	0.13
(1,325)	1:110:A:ALA:H	1:112:A:GLU:H	7	0.13
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	3	0.13
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	17	0.13
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	19	0.13
(1,311)	1:99:A:GLY:H	1:100:A:ALA:H	3	0.13
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	1	0.13
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	9	0.13
(1,305)	1:97:A:CYS:H	1:100:A:ALA:H	8	0.13
(1,304)	1:97:A:CYS:H	1:99:A:GLY:H	8	0.13
(1,297)	1:95:A:ALA:H	1:98:A:LEU:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:95:A:ALA:H	1:98:A:LEU:H	18	0.13
(1,290)	1:94:A:MET:H	1:95:A:ALA:H	15	0.13
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	1	0.13
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	14	0.13
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	1	0.13
(1,258)	1:78:A:VAL:HG11	1:79:A:GLN:H	7	0.13
(1,258)	1:78:A:VAL:HG12	1:79:A:GLN:H	7	0.13
(1,258)	1:78:A:VAL:HG13	1:79:A:GLN:H	7	0.13
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB1	8	0.13
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB2	8	0.13
(1,234)	1:68:A:LEU:HD11	1:73:A:ALA:HB3	8	0.13
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB1	8	0.13
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB2	8	0.13
(1,234)	1:68:A:LEU:HD12	1:73:A:ALA:HB3	8	0.13
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB1	8	0.13
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB2	8	0.13
(1,234)	1:68:A:LEU:HD13	1:73:A:ALA:HB3	8	0.13
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	3	0.13
(1,220)	1:66:A:ALA:H	1:76:A:CYS:H	16	0.13
(1,217)	1:66:A:ALA:H	1:67:A:SER:H	5	0.13
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	18	0.13
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	18	0.13
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	18	0.13
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	18	0.13
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	18	0.13
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	18	0.13
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	18	0.13
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	18	0.13
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	18	0.13
(1,146)	1:50:A:GLN:H	1:57:A:GLU:H	16	0.13
(1,145)	1:50:A:GLN:H	1:51:A:LEU:H	19	0.13
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	3	0.13
(1,136)	1:47:A:ALA:H	1:59:A:VAL:H	12	0.13
(1,131)	1:45:A:ASP:H	1:62:A:VAL:H	12	0.13
(1,118)	1:43:A:ASP:H	1:44:A:LEU:H	7	0.13
(1,115)	1:42:A:LEU:HD21	1:43:A:ASP:H	1	0.13
(1,115)	1:42:A:LEU:HD22	1:43:A:ASP:H	1	0.13
(1,115)	1:42:A:LEU:HD23	1:43:A:ASP:H	1	0.13
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	10	0.13
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	10	0.13
(1,95)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	10	0.13
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	7	0.13
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	16	0.13
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	16	0.13
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	2	0.13
(1,67)	1:28:A:ALA:HB1	1:17:B:TYR:HE1	17	0.13
(1,67)	1:28:A:ALA:HB1	1:17:B:TYR:HE2	17	0.13
(1,67)	1:28:A:ALA:HB2	1:17:B:TYR:HE1	17	0.13
(1,67)	1:28:A:ALA:HB2	1:17:B:TYR:HE2	17	0.13
(1,67)	1:28:A:ALA:HB3	1:17:B:TYR:HE1	17	0.13
(1,67)	1:28:A:ALA:HB3	1:17:B:TYR:HE2	17	0.13
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	12	0.13
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	12	0.13
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	1	0.13
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	8	0.13
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	10	0.13
(1,31)	1:18:A:THR:H	1:122:B:THR:H	12	0.13
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	4	0.13
(1,16)	1:14:A:GLN:H	1:83:A:ILE:H	1	0.13
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	5	0.12
(2,2)	1:40:C:VAL:O	2:290:F:TRP:NE1	9	0.12
(2,2)	1:40:C:VAL:O	2:290:F:TRP:NE1	18	0.12
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	17	0.12
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	17	0.12
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	17	0.12
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	17	0.12
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	17	0.12
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	17	0.12
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	17	0.12
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	17	0.12
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	17	0.12
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG21	16	0.12
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG22	16	0.12
(1,1705)	1:131:C:VAL:HG21	2:309:H:THR:HG23	16	0.12
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG21	16	0.12
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG22	16	0.12
(1,1705)	1:131:C:VAL:HG22	2:309:H:THR:HG23	16	0.12
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG21	16	0.12
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG22	16	0.12
(1,1705)	1:131:C:VAL:HG23	2:309:H:THR:HG23	16	0.12
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	7	0.12
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	7	0.12
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	7	0.12
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	7	0.12
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	7	0.12
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD11	5	0.12
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD12	5	0.12
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD13	5	0.12
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD21	5	0.12
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD22	5	0.12
(1,1684)	1:94:B:MET:HE1	2:278:H:LEU:HD23	5	0.12
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD11	5	0.12
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD12	5	0.12
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD13	5	0.12
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD21	5	0.12
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD22	5	0.12
(1,1684)	1:94:B:MET:HE2	2:278:H:LEU:HD23	5	0.12
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD11	5	0.12
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD12	5	0.12
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD13	5	0.12
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD21	5	0.12
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD22	5	0.12
(1,1684)	1:94:B:MET:HE3	2:278:H:LEU:HD23	5	0.12
(1,1683)	1:86:B:ILE:HD11	2:278:H:LEU:HD11	16	0.12
(1,1683)	1:86:B:ILE:HD11	2:278:H:LEU:HD12	16	0.12
(1,1683)	1:86:B:ILE:HD11	2:278:H:LEU:HD13	16	0.12
(1,1683)	1:86:B:ILE:HD11	2:278:H:LEU:HD21	16	0.12
(1,1683)	1:86:B:ILE:HD11	2:278:H:LEU:HD22	16	0.12
(1,1683)	1:86:B:ILE:HD11	2:278:H:LEU:HD23	16	0.12
(1,1683)	1:86:B:ILE:HD12	2:278:H:LEU:HD11	16	0.12
(1,1683)	1:86:B:ILE:HD12	2:278:H:LEU:HD12	16	0.12
(1,1683)	1:86:B:ILE:HD12	2:278:H:LEU:HD13	16	0.12
(1,1683)	1:86:B:ILE:HD12	2:278:H:LEU:HD21	16	0.12
(1,1683)	1:86:B:ILE:HD12	2:278:H:LEU:HD22	16	0.12
(1,1683)	1:86:B:ILE:HD12	2:278:H:LEU:HD23	16	0.12
(1,1683)	1:86:B:ILE:HD13	2:278:H:LEU:HD11	16	0.12
(1,1683)	1:86:B:ILE:HD13	2:278:H:LEU:HD12	16	0.12
(1,1683)	1:86:B:ILE:HD13	2:278:H:LEU:HD13	16	0.12
(1,1683)	1:86:B:ILE:HD13	2:278:H:LEU:HD21	16	0.12
(1,1683)	1:86:B:ILE:HD13	2:278:H:LEU:HD22	16	0.12
(1,1683)	1:86:B:ILE:HD13	2:278:H:LEU:HD23	16	0.12
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	2	0.12
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	2	0.12
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	2	0.12
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	2	0.12
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	2	0.12
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	11	0.12
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	11	0.12
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	11	0.12
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	11	0.12
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	11	0.12
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	11	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD11	3	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD12	3	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD13	3	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD21	3	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD22	3	0.12
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD23	3	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD11	3	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD12	3	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD13	3	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD21	3	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD22	3	0.12
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD23	3	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD11	3	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD12	3	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD13	3	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD21	3	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD22	3	0.12
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD23	3	0.12
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD11	11	0.12
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD12	11	0.12
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD13	11	0.12
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG21	14	0.12
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG22	14	0.12
(1,1657)	1:133:B:PHE:HE1	2:288:H:VAL:HG23	14	0.12
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG21	14	0.12
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG22	14	0.12
(1,1657)	1:133:B:PHE:HE2	2:288:H:VAL:HG23	14	0.12
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE1	9	0.12
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE2	9	0.12
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE3	9	0.12
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE1	9	0.12
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE2	9	0.12
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD11	20	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD12	20	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD13	20	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD21	20	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD22	20	0.12
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD23	20	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD11	20	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD12	20	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD13	20	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD21	20	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD22	20	0.12
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD23	20	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD11	20	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD12	20	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD13	20	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD21	20	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD22	20	0.12
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD23	20	0.12
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD11	11	0.12
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD12	11	0.12
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD13	11	0.12
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD21	11	0.12
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD22	11	0.12
(1,1629)	1:89:D:ILE:HD11	2:277:G:LEU:HD23	11	0.12
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD11	11	0.12
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD12	11	0.12
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD13	11	0.12
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD21	11	0.12
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD22	11	0.12
(1,1629)	1:89:D:ILE:HD12	2:277:G:LEU:HD23	11	0.12
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD11	11	0.12
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD12	11	0.12
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD13	11	0.12
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD21	11	0.12
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD22	11	0.12
(1,1629)	1:89:D:ILE:HD13	2:277:G:LEU:HD23	11	0.12
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	9	0.12
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	9	0.12
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	9	0.12
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	9	0.12
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	9	0.12
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	9	0.12
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	9	0.12
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	9	0.12
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	20	0.12
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	20	0.12
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	20	0.12
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	20	0.12
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	20	0.12
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	20	0.12
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	20	0.12
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	20	0.12
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	20	0.12
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG21	19	0.12
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG22	19	0.12
(1,1617)	1:118:D:VAL:HG11	2:296:G:THR:HG23	19	0.12
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG21	19	0.12
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG22	19	0.12
(1,1617)	1:118:D:VAL:HG12	2:296:G:THR:HG23	19	0.12
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG21	19	0.12
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG22	19	0.12
(1,1617)	1:118:D:VAL:HG13	2:296:G:THR:HG23	19	0.12
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG21	17	0.12
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG22	17	0.12
(1,1616)	1:74:D:PHE:HZ	2:296:G:THR:HG23	17	0.12
(1,1614)	1:126:D:LEU:HD11	2:290:G:TRP:HZ2	6	0.12
(1,1614)	1:126:D:LEU:HD12	2:290:G:TRP:HZ2	6	0.12
(1,1614)	1:126:D:LEU:HD13	2:290:G:TRP:HZ2	6	0.12
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD11	9	0.12
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD12	9	0.12
(1,1596)	1:36:C:TRP:HE3	2:301:F:ILE:HD13	9	0.12
(1,1594)	1:128:C:LEU:HD11	2:290:F:TRP:HE3	2	0.12
(1,1594)	1:128:C:LEU:HD12	2:290:F:TRP:HE3	2	0.12
(1,1594)	1:128:C:LEU:HD13	2:290:F:TRP:HE3	2	0.12
(1,1594)	1:128:C:LEU:HD21	2:290:F:TRP:HE3	2	0.12
(1,1594)	1:128:C:LEU:HD22	2:290:F:TRP:HE3	2	0.12
(1,1594)	1:128:C:LEU:HD23	2:290:F:TRP:HE3	2	0.12
(1,1594)	1:128:C:LEU:HD11	2:290:F:TRP:HE3	7	0.12
(1,1594)	1:128:C:LEU:HD12	2:290:F:TRP:HE3	7	0.12
(1,1594)	1:128:C:LEU:HD13	2:290:F:TRP:HE3	7	0.12
(1,1594)	1:128:C:LEU:HD21	2:290:F:TRP:HE3	7	0.12
(1,1594)	1:128:C:LEU:HD22	2:290:F:TRP:HE3	7	0.12
(1,1594)	1:128:C:LEU:HD23	2:290:F:TRP:HE3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD11	18	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD12	18	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD13	18	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD11	18	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD12	18	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD13	18	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD11	18	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD12	18	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD13	18	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD11	20	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD12	20	0.12
(1,1588)	1:42:C:LEU:HD11	2:291:F:LEU:HD13	20	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD11	20	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD12	20	0.12
(1,1588)	1:42:C:LEU:HD12	2:291:F:LEU:HD13	20	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD11	20	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD12	20	0.12
(1,1588)	1:42:C:LEU:HD13	2:291:F:LEU:HD13	20	0.12
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	5	0.12
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	5	0.12
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	5	0.12
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	5	0.12
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	5	0.12
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	5	0.12
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	9	0.12
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	9	0.12
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	9	0.12
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	9	0.12
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	9	0.12
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	9	0.12
(1,1584)	1:98:C:LEU:HD11	2:281:F:PHE:HZ	11	0.12
(1,1584)	1:98:C:LEU:HD12	2:281:F:PHE:HZ	11	0.12
(1,1584)	1:98:C:LEU:HD13	2:281:F:PHE:HZ	11	0.12
(1,1584)	1:98:C:LEU:HD21	2:281:F:PHE:HZ	11	0.12
(1,1584)	1:98:C:LEU:HD22	2:281:F:PHE:HZ	11	0.12
(1,1584)	1:98:C:LEU:HD23	2:281:F:PHE:HZ	11	0.12
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD11	1	0.12
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD12	1	0.12
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD13	1	0.12
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD21	1	0.12
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD22	1	0.12
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD23	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD11	1	0.12
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD12	1	0.12
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD13	1	0.12
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD21	1	0.12
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD22	1	0.12
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD23	1	0.12
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD11	1	0.12
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD12	1	0.12
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD13	1	0.12
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD21	1	0.12
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD22	1	0.12
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD23	1	0.12
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD11	1	0.12
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD12	1	0.12
(1,1568)	1:32:C:PHE:HE1	2:301:F:ILE:HD13	1	0.12
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD11	1	0.12
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD12	1	0.12
(1,1568)	1:32:C:PHE:HE2	2:301:F:ILE:HD13	1	0.12
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD11	19	0.12
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD12	19	0.12
(1,1567)	1:123:C:PHE:HE1	2:301:F:ILE:HD13	19	0.12
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD11	19	0.12
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD12	19	0.12
(1,1567)	1:123:C:PHE:HE2	2:301:F:ILE:HD13	19	0.12
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	20	0.12
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	20	0.12
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	20	0.12
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	20	0.12
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	20	0.12
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	20	0.12
(1,1549)	1:137:C:PHE:HD1	2:286:F:MET:HE1	8	0.12
(1,1549)	1:137:C:PHE:HD1	2:286:F:MET:HE2	8	0.12
(1,1549)	1:137:C:PHE:HD1	2:286:F:MET:HE3	8	0.12
(1,1549)	1:137:C:PHE:HD2	2:286:F:MET:HE1	8	0.12
(1,1549)	1:137:C:PHE:HD2	2:286:F:MET:HE2	8	0.12
(1,1549)	1:137:C:PHE:HD2	2:286:F:MET:HE3	8	0.12
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD11	17	0.12
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD12	17	0.12
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD13	17	0.12
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD21	17	0.12
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD22	17	0.12
(1,1529)	1:98:A:LEU:HD11	2:280:E:LEU:HD23	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD11	17	0.12
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD12	17	0.12
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD13	17	0.12
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD21	17	0.12
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD22	17	0.12
(1,1529)	1:98:A:LEU:HD12	2:280:E:LEU:HD23	17	0.12
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD11	17	0.12
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD12	17	0.12
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD13	17	0.12
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD21	17	0.12
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD22	17	0.12
(1,1529)	1:98:A:LEU:HD13	2:280:E:LEU:HD23	17	0.12
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD11	17	0.12
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD12	17	0.12
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD13	17	0.12
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD21	17	0.12
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD22	17	0.12
(1,1529)	1:98:A:LEU:HD21	2:280:E:LEU:HD23	17	0.12
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD11	17	0.12
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD12	17	0.12
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD13	17	0.12
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD21	17	0.12
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD22	17	0.12
(1,1529)	1:98:A:LEU:HD22	2:280:E:LEU:HD23	17	0.12
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD11	17	0.12
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD12	17	0.12
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD13	17	0.12
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD21	17	0.12
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD22	17	0.12
(1,1529)	1:98:A:LEU:HD23	2:280:E:LEU:HD23	17	0.12
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD11	13	0.12
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD12	13	0.12
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD13	13	0.12
(1,1482)	1:136:D:LEU:H	1:137:D:PHE:H	18	0.12
(1,1464)	1:131:D:VAL:H	1:133:D:PHE:H	20	0.12
(1,1458)	1:126:D:LEU:H	1:127:D:ASN:H	1	0.12
(1,1434)	1:113:D:CYS:H	1:116:D:SER:H	12	0.12
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	5	0.12
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	12	0.12
(1,1414)	1:100:D:ALA:H	1:102:D:CYS:H	10	0.12
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	13	0.12
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	18	0.12
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	2	0.12
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	10	0.12
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	18	0.12
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD21	2	0.12
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD22	2	0.12
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD23	2	0.12
(1,1216)	1:39:D:GLU:H	1:68:D:LEU:H	8	0.12
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	19	0.12
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	19	0.12
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	19	0.12
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	19	0.12
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	19	0.12
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	19	0.12
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	19	0.12
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	19	0.12
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	19	0.12
(1,1183)	1:28:D:ALA:H	1:31:D:VAL:H	14	0.12
(1,1176)	1:24:D:GLU:H	1:75:D:LEU:H	19	0.12
(1,1167)	1:22:D:SER:H	1:77:D:GLU:H	7	0.12
(1,1155)	1:17:D:TYR:H	1:81:D:GLY:H	11	0.12
(1,1147)	1:14:D:GLN:H	1:15:D:ARG:H	4	0.12
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	14	0.12
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	1	0.12
(1,1052)	1:100:C:ALA:H	1:102:C:CYS:H	18	0.12
(1,1038)	1:97:C:CYS:H	1:98:C:LEU:H	7	0.12
(1,1036)	1:96:C:HIS:H	1:98:C:LEU:H	14	0.12
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	9	0.12
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	9	0.12
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	9	0.12
(1,998)	1:78:C:VAL:HG11	1:79:C:GLN:H	10	0.12
(1,998)	1:78:C:VAL:HG12	1:79:C:GLN:H	10	0.12
(1,998)	1:78:C:VAL:HG13	1:79:C:GLN:H	10	0.12
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	4	0.12
(1,932)	1:59:C:VAL:H	1:60:C:LEU:H	2	0.12
(1,913)	1:56:C:TYR:H	1:85:C:SER:H	13	0.12
(1,909)	1:55:C:VAL:H	1:86:C:ILE:H	20	0.12
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	13	0.12
(1,854)	1:41:C:LYS:H	1:65:C:THR:H	15	0.12
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	15	0.12
(1,785)	1:19:C:LYS:H	1:20:C:ASP:H	3	0.12
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB1	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB2	9	0.12
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB3	9	0.12
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB1	9	0.12
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB2	9	0.12
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB3	9	0.12
(1,765)	1:14:C:GLN:H	1:15:C:ARG:H	18	0.12
(1,762)	1:12:C:GLN:H	1:13:C:ILE:H	8	0.12
(1,708)	1:118:B:VAL:HG21	1:121:B:GLY:H	6	0.12
(1,708)	1:118:B:VAL:HG22	1:121:B:GLY:H	6	0.12
(1,708)	1:118:B:VAL:HG23	1:121:B:GLY:H	6	0.12
(1,697)	1:115:B:THR:H	1:117:B:MET:H	8	0.12
(1,697)	1:115:B:THR:H	1:117:B:MET:H	18	0.12
(1,696)	1:115:B:THR:H	1:116:B:SER:H	19	0.12
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	10	0.12
(1,682)	1:110:B:ALA:H	1:112:B:GLU:H	4	0.12
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	12	0.12
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	20	0.12
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	1	0.12
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	17	0.12
(1,658)	1:97:B:CYS:H	1:99:B:GLY:H	3	0.12
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD21	9	0.12
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD22	9	0.12
(1,648)	1:94:B:MET:HE1	1:98:B:LEU:HD23	9	0.12
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD21	9	0.12
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD22	9	0.12
(1,648)	1:94:B:MET:HE2	1:98:B:LEU:HD23	9	0.12
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD21	9	0.12
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD22	9	0.12
(1,648)	1:94:B:MET:HE3	1:98:B:LEU:HD23	9	0.12
(1,646)	1:94:B:MET:H	1:96:B:HIS:H	10	0.12
(1,644)	1:93:B:GLN:H	1:96:B:HIS:H	16	0.12
(1,632)	1:88:B:GLY:H	1:89:B:ILE:H	8	0.12
(1,618)	1:79:B:GLN:H	1:80:B:GLN:H	3	0.12
(1,604)	1:73:B:ALA:H	1:74:B:PHE:H	18	0.12
(1,572)	1:62:B:VAL:H	1:80:B:GLN:H	6	0.12
(1,565)	1:60:B:LEU:H	1:82:B:GLY:H	20	0.12
(1,557)	1:59:B:VAL:H	1:60:B:LEU:H	15	0.12
(1,557)	1:59:B:VAL:H	1:60:B:LEU:H	18	0.12
(1,554)	1:58:B:VAL:HG11	1:98:B:LEU:HD11	19	0.12
(1,554)	1:58:B:VAL:HG11	1:98:B:LEU:HD12	19	0.12
(1,554)	1:58:B:VAL:HG11	1:98:B:LEU:HD13	19	0.12
(1,554)	1:58:B:VAL:HG12	1:98:B:LEU:HD11	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,554)	1:58:B:VAL:HG12	1:98:B:LEU:HD12	19	0.12
(1,554)	1:58:B:VAL:HG12	1:98:B:LEU:HD13	19	0.12
(1,554)	1:58:B:VAL:HG13	1:98:B:LEU:HD11	19	0.12
(1,554)	1:58:B:VAL:HG13	1:98:B:LEU:HD12	19	0.12
(1,554)	1:58:B:VAL:HG13	1:98:B:LEU:HD13	19	0.12
(1,553)	1:58:B:VAL:HG11	1:59:B:VAL:H	11	0.12
(1,553)	1:58:B:VAL:HG12	1:59:B:VAL:H	11	0.12
(1,553)	1:58:B:VAL:HG13	1:59:B:VAL:H	11	0.12
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	17	0.12
(1,499)	1:44:B:LEU:HD11	1:45:B:ASP:H	5	0.12
(1,499)	1:44:B:LEU:HD12	1:45:B:ASP:H	5	0.12
(1,499)	1:44:B:LEU:HD13	1:45:B:ASP:H	5	0.12
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	12	0.12
(1,480)	1:39:B:GLU:H	1:69:B:GLY:H	13	0.12
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD21	4	0.12
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD22	4	0.12
(1,476)	1:37:B:GLN:H	1:68:B:LEU:HD23	4	0.12
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD21	8	0.12
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD22	8	0.12
(1,471)	1:35:B:ASP:H	1:68:B:LEU:HD23	8	0.12
(1,460)	1:31:B:VAL:HG21	1:36:B:TRP:H	11	0.12
(1,460)	1:31:B:VAL:HG22	1:36:B:TRP:H	11	0.12
(1,460)	1:31:B:VAL:HG23	1:36:B:TRP:H	11	0.12
(1,451)	1:28:B:ALA:H	1:30:B:HIS:H	10	0.12
(1,413)	1:12:B:GLN:H	1:13:B:ILE:H	13	0.12
(1,413)	1:12:B:GLN:H	1:13:B:ILE:H	17	0.12
(1,396)	1:138:A:MET:H	1:141:A:LEU:H	2	0.12
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	16	0.12
(1,381)	1:134:A:ASP:H	1:136:A:LEU:H	9	0.12
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	7	0.12
(1,360)	1:122:A:THR:H	1:18:B:THR:H	4	0.12
(1,360)	1:122:A:THR:H	1:18:B:THR:H	8	0.12
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	2	0.12
(1,324)	1:110:A:ALA:H	1:111:A:ARG:H	15	0.12
(1,310)	1:98:A:LEU:H	1:102:A:CYS:H	2	0.12
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	1	0.12
(1,305)	1:97:A:CYS:H	1:100:A:ALA:H	20	0.12
(1,301)	1:96:A:HIS:H	1:98:A:LEU:H	7	0.12
(1,290)	1:94:A:MET:H	1:95:A:ALA:H	3	0.12
(1,290)	1:94:A:MET:H	1:95:A:ALA:H	7	0.12
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	18	0.12
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:66:A:ALA:H	1:67:A:SER:H	20	0.12
(1,177)	1:58:A:VAL:H	1:84:A:PHE:H	16	0.12
(1,165)	1:55:A:VAL:H	1:56:A:TYR:H	10	0.12
(1,155)	1:52:A:ALA:H	1:55:A:VAL:H	10	0.12
(1,143)	1:49:A:SER:H	1:58:A:VAL:H	12	0.12
(1,97)	1:39:A:GLU:H	1:40:A:VAL:H	8	0.12
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	2	0.12
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	2	0.12
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	19	0.12
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	19	0.12
(1,84)	1:32:A:PHE:H	1:33:A:GLN:H	10	0.12
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	3	0.12
(1,69)	1:30:A:HIS:H	1:32:A:PHE:H	3	0.12
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	7	0.12
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	7	0.12
(1,51)	1:23:A:PHE:HD1	1:24:A:GLU:H	19	0.12
(1,51)	1:23:A:PHE:HD2	1:24:A:GLU:H	19	0.12
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	9	0.12
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	15	0.12
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	17	0.12
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	9	0.12
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	14	0.12
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB1	3	0.12
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB2	3	0.12
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB3	3	0.12
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB1	3	0.12
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB2	3	0.12
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB3	3	0.12
(2,4)	1:40:B:VAL:O	2:290:H:TRP:NE1	2	0.11
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD11	10	0.11
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD12	10	0.11
(1,1702)	1:36:B:TRP:HE3	2:301:H:ILE:HD13	10	0.11
(1,1700)	1:128:B:LEU:HD11	2:290:H:TRP:HE3	12	0.11
(1,1700)	1:128:B:LEU:HD12	2:290:H:TRP:HE3	12	0.11
(1,1700)	1:128:B:LEU:HD13	2:290:H:TRP:HE3	12	0.11
(1,1700)	1:128:B:LEU:HD21	2:290:H:TRP:HE3	12	0.11
(1,1700)	1:128:B:LEU:HD22	2:290:H:TRP:HE3	12	0.11
(1,1700)	1:128:B:LEU:HD23	2:290:H:TRP:HE3	12	0.11
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD11	20	0.11
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD12	20	0.11
(1,1679)	1:31:B:VAL:HG11	2:301:H:ILE:HD13	20	0.11
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD11	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD12	20	0.11
(1,1679)	1:31:B:VAL:HG12	2:301:H:ILE:HD13	20	0.11
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD11	20	0.11
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD12	20	0.11
(1,1679)	1:31:B:VAL:HG13	2:301:H:ILE:HD13	20	0.11
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD11	9	0.11
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD12	9	0.11
(1,1675)	1:36:B:TRP:HH2	2:301:H:ILE:HD13	9	0.11
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	1	0.11
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	1	0.11
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	1	0.11
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	1	0.11
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	1	0.11
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	1	0.11
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	14	0.11
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	14	0.11
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	14	0.11
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	14	0.11
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	14	0.11
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	14	0.11
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	6	0.11
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	6	0.11
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	6	0.11
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	6	0.11
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	6	0.11
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	6	0.11
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD1	8	0.11
(1,1671)	1:68:B:LEU:HD21	2:297:H:TYR:HD2	8	0.11
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD1	8	0.11
(1,1671)	1:68:B:LEU:HD22	2:297:H:TYR:HD2	8	0.11
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD1	8	0.11
(1,1671)	1:68:B:LEU:HD23	2:297:H:TYR:HD2	8	0.11
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD11	5	0.11
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD12	5	0.11
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD13	5	0.11
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD21	5	0.11
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD22	5	0.11
(1,1665)	1:58:B:VAL:HG21	2:278:H:LEU:HD23	5	0.11
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD11	5	0.11
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD12	5	0.11
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD13	5	0.11
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD21	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD22	5	0.11
(1,1665)	1:58:B:VAL:HG22	2:278:H:LEU:HD23	5	0.11
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD11	5	0.11
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD12	5	0.11
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD13	5	0.11
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD21	5	0.11
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD22	5	0.11
(1,1665)	1:58:B:VAL:HG23	2:278:H:LEU:HD23	5	0.11
(1,1659)	1:60:B:LEU:HD21	2:281:H:PHE:HZ	16	0.11
(1,1659)	1:60:B:LEU:HD22	2:281:H:PHE:HZ	16	0.11
(1,1659)	1:60:B:LEU:HD23	2:281:H:PHE:HZ	16	0.11
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	7	0.11
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	7	0.11
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	7	0.11
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	7	0.11
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	7	0.11
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	7	0.11
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	7	0.11
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	7	0.11
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	7	0.11
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG21	19	0.11
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG22	19	0.11
(1,1652)	1:131:A:VAL:HG21	2:309:G:THR:HG23	19	0.11
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG21	19	0.11
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG22	19	0.11
(1,1652)	1:131:A:VAL:HG22	2:309:G:THR:HG23	19	0.11
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG21	19	0.11
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG22	19	0.11
(1,1652)	1:131:A:VAL:HG23	2:309:G:THR:HG23	19	0.11
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD11	19	0.11
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD12	19	0.11
(1,1649)	1:36:D:TRP:HE3	2:301:G:ILE:HD13	19	0.11
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE1	13	0.11
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE2	13	0.11
(1,1643)	1:133:D:PHE:HE1	2:286:G:MET:HE3	13	0.11
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE1	13	0.11
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE2	13	0.11
(1,1643)	1:133:D:PHE:HE2	2:286:G:MET:HE3	13	0.11
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD11	13	0.11
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD12	13	0.11
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD13	13	0.11
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD21	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD22	13	0.11
(1,1631)	1:94:D:MET:HE1	2:278:G:LEU:HD23	13	0.11
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD11	13	0.11
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD12	13	0.11
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD13	13	0.11
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD21	13	0.11
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD22	13	0.11
(1,1631)	1:94:D:MET:HE2	2:278:G:LEU:HD23	13	0.11
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD11	13	0.11
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD12	13	0.11
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD13	13	0.11
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD21	13	0.11
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD22	13	0.11
(1,1631)	1:94:D:MET:HE3	2:278:G:LEU:HD23	13	0.11
(1,1614)	1:126:D:LEU:HD11	2:290:G:TRP:HZ2	18	0.11
(1,1614)	1:126:D:LEU:HD12	2:290:G:TRP:HZ2	18	0.11
(1,1614)	1:126:D:LEU:HD13	2:290:G:TRP:HZ2	18	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG21	1	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG22	1	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG23	1	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG21	1	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG22	1	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG23	1	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG21	1	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG22	1	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG23	1	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG21	11	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG22	11	0.11
(1,1600)	1:129:B:ALA:HB1	2:309:F:THR:HG23	11	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG21	11	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG22	11	0.11
(1,1600)	1:129:B:ALA:HB2	2:309:F:THR:HG23	11	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG21	11	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG22	11	0.11
(1,1600)	1:129:B:ALA:HB3	2:309:F:THR:HG23	11	0.11
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD11	9	0.11
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD12	9	0.11
(1,1585)	1:128:C:LEU:HD11	2:291:F:LEU:HD13	9	0.11
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD11	9	0.11
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD12	9	0.11
(1,1585)	1:128:C:LEU:HD12	2:291:F:LEU:HD13	9	0.11
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD11	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD12	9	0.11
(1,1585)	1:128:C:LEU:HD13	2:291:F:LEU:HD13	9	0.11
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	1	0.11
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	1	0.11
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	1	0.11
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	1	0.11
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	1	0.11
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	1	0.11
(1,1560)	1:129:C:ALA:HB1	2:290:F:TRP:HZ3	19	0.11
(1,1560)	1:129:C:ALA:HB2	2:290:F:TRP:HZ3	19	0.11
(1,1560)	1:129:C:ALA:HB3	2:290:F:TRP:HZ3	19	0.11
(1,1551)	1:133:C:PHE:HE1	2:288:F:VAL:HG21	8	0.11
(1,1551)	1:133:C:PHE:HE1	2:288:F:VAL:HG22	8	0.11
(1,1551)	1:133:C:PHE:HE1	2:288:F:VAL:HG23	8	0.11
(1,1551)	1:133:C:PHE:HE2	2:288:F:VAL:HG21	8	0.11
(1,1551)	1:133:C:PHE:HE2	2:288:F:VAL:HG22	8	0.11
(1,1551)	1:133:C:PHE:HE2	2:288:F:VAL:HG23	8	0.11
(1,1541)	1:128:A:LEU:HD11	2:290:E:TRP:HE3	9	0.11
(1,1541)	1:128:A:LEU:HD12	2:290:E:TRP:HE3	9	0.11
(1,1541)	1:128:A:LEU:HD13	2:290:E:TRP:HE3	9	0.11
(1,1541)	1:128:A:LEU:HD21	2:290:E:TRP:HE3	9	0.11
(1,1541)	1:128:A:LEU:HD22	2:290:E:TRP:HE3	9	0.11
(1,1541)	1:128:A:LEU:HD23	2:290:E:TRP:HE3	9	0.11
(1,1533)	1:131:A:VAL:HG21	2:291:E:LEU:HD11	20	0.11
(1,1533)	1:131:A:VAL:HG21	2:291:E:LEU:HD12	20	0.11
(1,1533)	1:131:A:VAL:HG21	2:291:E:LEU:HD13	20	0.11
(1,1533)	1:131:A:VAL:HG22	2:291:E:LEU:HD11	20	0.11
(1,1533)	1:131:A:VAL:HG22	2:291:E:LEU:HD12	20	0.11
(1,1533)	1:131:A:VAL:HG22	2:291:E:LEU:HD13	20	0.11
(1,1533)	1:131:A:VAL:HG23	2:291:E:LEU:HD11	20	0.11
(1,1533)	1:131:A:VAL:HG23	2:291:E:LEU:HD12	20	0.11
(1,1533)	1:131:A:VAL:HG23	2:291:E:LEU:HD13	20	0.11
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD11	16	0.11
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD12	16	0.11
(1,1520)	1:31:A:VAL:HG11	2:301:E:ILE:HD13	16	0.11
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD11	16	0.11
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD12	16	0.11
(1,1520)	1:31:A:VAL:HG12	2:301:E:ILE:HD13	16	0.11
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD11	16	0.11
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD12	16	0.11
(1,1520)	1:31:A:VAL:HG13	2:301:E:ILE:HD13	16	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG11	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG12	13	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG13	13	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG11	13	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG12	13	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG13	13	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG11	13	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG12	13	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG13	13	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG11	16	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG12	16	0.11
(1,1518)	1:129:A:ALA:HB1	2:288:E:VAL:HG13	16	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG11	16	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG12	16	0.11
(1,1518)	1:129:A:ALA:HB2	2:288:E:VAL:HG13	16	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG11	16	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG12	16	0.11
(1,1518)	1:129:A:ALA:HB3	2:288:E:VAL:HG13	16	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD11	4	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD12	4	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD13	4	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD11	9	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD12	9	0.11
(1,1505)	1:137:A:PHE:HZ	2:280:E:LEU:HD13	9	0.11
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	14	0.11
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	14	0.11
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	14	0.11
(1,1475)	1:135:D:ALA:H	1:136:D:LEU:H	20	0.11
(1,1469)	1:133:D:PHE:H	1:135:D:ALA:H	7	0.11
(1,1455)	1:121:D:GLY:H	1:123:D:PHE:H	11	0.11
(1,1424)	1:110:D:ALA:H	1:111:D:ARG:H	7	0.11
(1,1392)	1:94:D:MET:HE1	1:95:D:ALA:H	11	0.11
(1,1392)	1:94:D:MET:HE2	1:95:D:ALA:H	11	0.11
(1,1392)	1:94:D:MET:HE3	1:95:D:ALA:H	11	0.11
(1,1390)	1:94:D:MET:H	1:96:D:HIS:H	15	0.11
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	8	0.11
(1,1373)	1:87:D:ALA:H	1:88:D:GLY:H	15	0.11
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	8	0.11
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	15	0.11
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	16	0.11
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	10	0.11
(1,1325)	1:68:D:LEU:H	1:69:D:GLY:H	14	0.11
(1,1304)	1:64:D:VAL:H	1:65:D:THR:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:49:D:SER:H	1:59:D:VAL:H	1	0.11
(1,1212)	1:36:D:TRP:HE3	1:37:D:GLN:H	1	0.11
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD11	8	0.11
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD12	8	0.11
(1,1210)	1:36:D:TRP:H	1:68:D:LEU:HD13	8	0.11
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	20	0.11
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	20	0.11
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	20	0.11
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	20	0.11
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	20	0.11
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	20	0.11
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	20	0.11
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	20	0.11
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	20	0.11
(1,1185)	1:30:D:HIS:H	1:31:D:VAL:H	8	0.11
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB1	20	0.11
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB2	20	0.11
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB3	20	0.11
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB1	20	0.11
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB2	20	0.11
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB3	20	0.11
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB1	20	0.11
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB2	20	0.11
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB3	20	0.11
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	3	0.11
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	4	0.11
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	8	0.11
(1,1161)	1:19:D:LYS:H	1:80:D:GLN:H	11	0.11
(1,1155)	1:17:D:TYR:H	1:81:D:GLY:H	3	0.11
(1,1148)	1:14:D:GLN:H	1:83:D:ILE:H	3	0.11
(1,1136)	1:10:D:THR:H	1:87:D:ALA:H	10	0.11
(1,1118)	1:135:C:ALA:H	1:138:C:MET:H	19	0.11
(1,1104)	1:128:C:LEU:HD11	1:129:C:ALA:H	5	0.11
(1,1104)	1:128:C:LEU:HD12	1:129:C:ALA:H	5	0.11
(1,1104)	1:128:C:LEU:HD13	1:129:C:ALA:H	5	0.11
(1,1097)	1:126:C:LEU:H	1:127:C:ASN:H	14	0.11
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	5	0.11
(1,1082)	1:117:C:MET:H	1:119:C:SER:H	16	0.11
(1,1060)	1:110:C:ALA:H	1:111:C:ARG:H	17	0.11
(1,1046)	1:98:C:LEU:HD11	1:99:C:GLY:H	9	0.11
(1,1046)	1:98:C:LEU:HD12	1:99:C:GLY:H	9	0.11
(1,1046)	1:98:C:LEU:HD13	1:99:C:GLY:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:98:C:LEU:H	1:100:C:ALA:H	17	0.11
(1,1033)	1:95:C:ALA:H	1:98:C:LEU:H	6	0.11
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	5	0.11
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	14	0.11
(1,1022)	1:91:C:GLY:H	1:95:C:ALA:H	13	0.11
(1,1019)	1:90:C:GLU:H	1:94:C:MET:H	9	0.11
(1,1014)	1:87:C:ALA:H	1:89:C:ILE:H	9	0.11
(1,1007)	1:82:C:GLY:H	1:83:C:ILE:H	19	0.11
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	19	0.11
(1,951)	1:64:C:VAL:H	1:65:C:THR:H	18	0.11
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	3	0.11
(1,932)	1:59:C:VAL:H	1:60:C:LEU:H	18	0.11
(1,869)	1:44:C:LEU:H	1:63:C:THR:H	16	0.11
(1,836)	1:34:C:LYS:H	1:36:C:TRP:HZ3	4	0.11
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	16	0.11
(1,801)	1:23:C:PHE:H	1:24:C:GLU:H	18	0.11
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB1	3	0.11
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB2	3	0.11
(1,779)	1:17:C:TYR:HE1	1:28:D:ALA:HB3	3	0.11
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB1	3	0.11
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB2	3	0.11
(1,779)	1:17:C:TYR:HE2	1:28:D:ALA:HB3	3	0.11
(1,768)	1:14:C:GLN:H	1:85:C:SER:H	14	0.11
(1,758)	1:11:C:PHE:HE1	1:12:C:GLN:H	9	0.11
(1,758)	1:11:C:PHE:HE2	1:12:C:GLN:H	9	0.11
(1,729)	1:133:B:PHE:H	1:135:B:ALA:H	1	0.11
(1,718)	1:126:B:LEU:HD21	1:127:B:ASN:H	15	0.11
(1,718)	1:126:B:LEU:HD22	1:127:B:ASN:H	15	0.11
(1,718)	1:126:B:LEU:HD23	1:127:B:ASN:H	15	0.11
(1,698)	1:116:B:SER:H	1:117:B:MET:H	3	0.11
(1,697)	1:115:B:THR:H	1:117:B:MET:H	14	0.11
(1,696)	1:115:B:THR:H	1:116:B:SER:H	2	0.11
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	3	0.11
(1,682)	1:110:B:ALA:H	1:112:B:GLU:H	7	0.11
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	1	0.11
(1,670)	1:100:B:ALA:H	1:101:B:TYR:H	18	0.11
(1,668)	1:99:B:GLY:H	1:101:B:TYR:H	11	0.11
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	6	0.11
(1,657)	1:97:B:CYS:H	1:98:B:LEU:H	7	0.11
(1,657)	1:97:B:CYS:H	1:98:B:LEU:H	20	0.11
(1,655)	1:96:B:HIS:H	1:98:B:LEU:H	19	0.11
(1,640)	1:92:B:THR:H	1:94:B:MET:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,640)	1:92:B:THR:H	1:94:B:MET:H	15	0.11
(1,630)	1:87:B:ALA:H	1:89:B:ILE:H	15	0.11
(1,597)	1:68:B:LEU:H	1:74:B:PHE:H	2	0.11
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB1	3	0.11
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB2	3	0.11
(1,596)	1:68:B:LEU:H	1:73:B:ALA:HB3	3	0.11
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	3	0.11
(1,586)	1:66:B:ALA:H	1:76:B:CYS:H	15	0.11
(1,553)	1:58:B:VAL:HG11	1:59:B:VAL:H	16	0.11
(1,553)	1:58:B:VAL:HG12	1:59:B:VAL:H	16	0.11
(1,553)	1:58:B:VAL:HG13	1:59:B:VAL:H	16	0.11
(1,508)	1:47:B:ALA:H	1:48:B:SER:H	6	0.11
(1,506)	1:45:B:ASP:H	1:63:B:THR:H	9	0.11
(1,489)	1:42:B:LEU:HD11	1:128:B:LEU:HD11	10	0.11
(1,489)	1:42:B:LEU:HD11	1:128:B:LEU:HD12	10	0.11
(1,489)	1:42:B:LEU:HD11	1:128:B:LEU:HD13	10	0.11
(1,489)	1:42:B:LEU:HD12	1:128:B:LEU:HD11	10	0.11
(1,489)	1:42:B:LEU:HD12	1:128:B:LEU:HD12	10	0.11
(1,489)	1:42:B:LEU:HD12	1:128:B:LEU:HD13	10	0.11
(1,489)	1:42:B:LEU:HD13	1:128:B:LEU:HD11	10	0.11
(1,489)	1:42:B:LEU:HD13	1:128:B:LEU:HD12	10	0.11
(1,489)	1:42:B:LEU:HD13	1:128:B:LEU:HD13	10	0.11
(1,468)	1:34:B:LYS:H	1:35:B:ASP:H	1	0.11
(1,462)	1:31:B:VAL:HG21	1:123:B:PHE:HE1	15	0.11
(1,462)	1:31:B:VAL:HG21	1:123:B:PHE:HE2	15	0.11
(1,462)	1:31:B:VAL:HG22	1:123:B:PHE:HE1	15	0.11
(1,462)	1:31:B:VAL:HG22	1:123:B:PHE:HE2	15	0.11
(1,462)	1:31:B:VAL:HG23	1:123:B:PHE:HE1	15	0.11
(1,462)	1:31:B:VAL:HG23	1:123:B:PHE:HE2	15	0.11
(1,455)	1:31:B:VAL:H	1:32:B:PHE:H	19	0.11
(1,450)	1:27:B:ASN:H	1:28:B:ALA:H	4	0.11
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	2	0.11
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	2	0.11
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	2	0.11
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	2	0.11
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	2	0.11
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	2	0.11
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	2	0.11
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	2	0.11
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	2	0.11
(1,421)	1:15:B:ARG:H	1:83:B:ILE:H	5	0.11
(1,418)	1:14:B:GLN:H	1:83:B:ILE:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	20	0.11
(1,410)	1:11:B:PHE:HD1	1:12:B:GLN:H	12	0.11
(1,410)	1:11:B:PHE:HD2	1:12:B:GLN:H	12	0.11
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	19	0.11
(1,392)	1:137:A:PHE:H	1:140:A:TYR:H	15	0.11
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	1	0.11
(1,390)	1:137:A:PHE:H	1:138:A:MET:H	6	0.11
(1,378)	1:133:A:PHE:H	1:136:A:LEU:H	11	0.11
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	14	0.11
(1,370)	1:128:A:LEU:HD21	1:129:A:ALA:H	8	0.11
(1,370)	1:128:A:LEU:HD22	1:129:A:ALA:H	8	0.11
(1,370)	1:128:A:LEU:HD23	1:129:A:ALA:H	8	0.11
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	5	0.11
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	16	0.11
(1,322)	1:109:A:TYR:H	1:111:A:ARG:H	4	0.11
(1,309)	1:98:A:LEU:H	1:101:A:TYR:H	12	0.11
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	13	0.11
(1,307)	1:98:A:LEU:H	1:99:A:GLY:H	14	0.11
(1,297)	1:95:A:ALA:H	1:98:A:LEU:H	10	0.11
(1,285)	1:92:A:THR:H	1:94:A:MET:H	10	0.11
(1,285)	1:92:A:THR:H	1:94:A:MET:H	13	0.11
(1,275)	1:87:A:ALA:H	1:89:A:ILE:H	19	0.11
(1,272)	1:85:A:SER:H	1:86:A:ILE:H	11	0.11
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	6	0.11
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	12	0.11
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE1	1	0.11
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE2	1	0.11
(1,256)	1:77:A:GLU:H	1:117:A:MET:HE3	1	0.11
(1,230)	1:68:A:LEU:H	1:70:A:GLU:H	6	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	7	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	7	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	7	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	7	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	7	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	7	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	7	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	7	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	7	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	10	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	10	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	10	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	10	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	10	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	10	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	10	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	10	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	14	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	14	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	14	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	14	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	14	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	14	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	14	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	14	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	14	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD21	20	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD22	20	0.11
(1,212)	1:64:A:VAL:HG11	1:126:A:LEU:HD23	20	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD21	20	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD22	20	0.11
(1,212)	1:64:A:VAL:HG12	1:126:A:LEU:HD23	20	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD21	20	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD22	20	0.11
(1,212)	1:64:A:VAL:HG13	1:126:A:LEU:HD23	20	0.11
(1,198)	1:62:A:VAL:H	1:63:A:THR:H	11	0.11
(1,198)	1:62:A:VAL:H	1:63:A:THR:H	17	0.11
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD1	8	0.11
(1,166)	1:55:A:VAL:H	1:56:A:TYR:HD2	8	0.11
(1,120)	1:43:A:ASP:H	1:65:A:THR:H	7	0.11
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD21	10	0.11
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD22	10	0.11
(1,104)	1:40:A:VAL:HG11	1:126:A:LEU:HD23	10	0.11
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD21	10	0.11
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD22	10	0.11
(1,104)	1:40:A:VAL:HG12	1:126:A:LEU:HD23	10	0.11
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD21	10	0.11
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD22	10	0.11
(1,104)	1:40:A:VAL:HG13	1:126:A:LEU:HD23	10	0.11
(1,87)	1:32:A:PHE:HD1	1:36:A:TRP:HZ3	13	0.11
(1,87)	1:32:A:PHE:HD2	1:36:A:TRP:HZ3	13	0.11
(1,86)	1:32:A:PHE:HD1	1:33:A:GLN:H	15	0.11
(1,86)	1:32:A:PHE:HD2	1:33:A:GLN:H	15	0.11
(1,84)	1:32:A:PHE:H	1:33:A:GLN:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:31:A:VAL:H	1:34:A:LYS:H	12	0.11
(1,53)	1:23:A:PHE:HE1	1:24:A:GLU:H	13	0.11
(1,53)	1:23:A:PHE:HE2	1:24:A:GLU:H	13	0.11
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	7	0.11
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	14	0.11
(1,35)	1:19:A:LYS:H	1:80:A:GLN:H	7	0.11
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	3	0.11
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	7	0.11
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	16	0.11
(1,32)	1:19:A:LYS:H	1:20:A:ASP:H	20	0.11
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB1	2	0.11
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB2	2	0.11
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB3	2	0.11
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB1	2	0.11
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB2	2	0.11
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB3	2	0.11
(1,24)	1:17:A:TYR:H	1:81:A:GLY:H	20	0.11
(1,15)	1:14:A:GLN:H	1:15:A:ARG:H	13	0.11
(1,3)	1:10:A:THR:H	1:87:A:ALA:H	5	0.11
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG21	11	0.1
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG22	11	0.1
(1,1706)	1:129:C:ALA:HB1	2:309:H:THR:HG23	11	0.1
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG21	11	0.1
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG22	11	0.1
(1,1706)	1:129:C:ALA:HB2	2:309:H:THR:HG23	11	0.1
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG21	11	0.1
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG22	11	0.1
(1,1706)	1:129:C:ALA:HB3	2:309:H:THR:HG23	11	0.1
(1,1696)	1:133:B:PHE:HE1	2:286:H:MET:HE1	17	0.1
(1,1696)	1:133:B:PHE:HE1	2:286:H:MET:HE2	17	0.1
(1,1696)	1:133:B:PHE:HE1	2:286:H:MET:HE3	17	0.1
(1,1696)	1:133:B:PHE:HE2	2:286:H:MET:HE1	17	0.1
(1,1696)	1:133:B:PHE:HE2	2:286:H:MET:HE2	17	0.1
(1,1696)	1:133:B:PHE:HE2	2:286:H:MET:HE3	17	0.1
(1,1690)	1:98:B:LEU:HD11	2:281:H:PHE:HZ	6	0.1
(1,1690)	1:98:B:LEU:HD12	2:281:H:PHE:HZ	6	0.1
(1,1690)	1:98:B:LEU:HD13	2:281:H:PHE:HZ	6	0.1
(1,1690)	1:98:B:LEU:HD21	2:281:H:PHE:HZ	6	0.1
(1,1690)	1:98:B:LEU:HD22	2:281:H:PHE:HZ	6	0.1
(1,1690)	1:98:B:LEU:HD23	2:281:H:PHE:HZ	6	0.1
(1,1682)	1:89:B:ILE:HD11	2:277:H:LEU:HD11	3	0.1
(1,1682)	1:89:B:ILE:HD11	2:277:H:LEU:HD12	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:89:B:ILE:HD11	2:277:H:LEU:HD13	3	0.1
(1,1682)	1:89:B:ILE:HD11	2:277:H:LEU:HD21	3	0.1
(1,1682)	1:89:B:ILE:HD11	2:277:H:LEU:HD22	3	0.1
(1,1682)	1:89:B:ILE:HD11	2:277:H:LEU:HD23	3	0.1
(1,1682)	1:89:B:ILE:HD12	2:277:H:LEU:HD11	3	0.1
(1,1682)	1:89:B:ILE:HD12	2:277:H:LEU:HD12	3	0.1
(1,1682)	1:89:B:ILE:HD12	2:277:H:LEU:HD13	3	0.1
(1,1682)	1:89:B:ILE:HD12	2:277:H:LEU:HD21	3	0.1
(1,1682)	1:89:B:ILE:HD12	2:277:H:LEU:HD22	3	0.1
(1,1682)	1:89:B:ILE:HD12	2:277:H:LEU:HD23	3	0.1
(1,1682)	1:89:B:ILE:HD13	2:277:H:LEU:HD11	3	0.1
(1,1682)	1:89:B:ILE:HD13	2:277:H:LEU:HD12	3	0.1
(1,1682)	1:89:B:ILE:HD13	2:277:H:LEU:HD13	3	0.1
(1,1682)	1:89:B:ILE:HD13	2:277:H:LEU:HD21	3	0.1
(1,1682)	1:89:B:ILE:HD13	2:277:H:LEU:HD22	3	0.1
(1,1682)	1:89:B:ILE:HD13	2:277:H:LEU:HD23	3	0.1
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD11	4	0.1
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD12	4	0.1
(1,1673)	1:123:B:PHE:HE1	2:301:H:ILE:HD13	4	0.1
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD11	4	0.1
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD12	4	0.1
(1,1673)	1:123:B:PHE:HE2	2:301:H:ILE:HD13	4	0.1
(1,1670)	1:118:B:VAL:HG11	2:296:H:THR:HG21	10	0.1
(1,1670)	1:118:B:VAL:HG11	2:296:H:THR:HG22	10	0.1
(1,1670)	1:118:B:VAL:HG11	2:296:H:THR:HG23	10	0.1
(1,1670)	1:118:B:VAL:HG12	2:296:H:THR:HG21	10	0.1
(1,1670)	1:118:B:VAL:HG12	2:296:H:THR:HG22	10	0.1
(1,1670)	1:118:B:VAL:HG12	2:296:H:THR:HG23	10	0.1
(1,1670)	1:118:B:VAL:HG13	2:296:H:THR:HG21	10	0.1
(1,1670)	1:118:B:VAL:HG13	2:296:H:THR:HG22	10	0.1
(1,1670)	1:118:B:VAL:HG13	2:296:H:THR:HG23	10	0.1
(1,1666)	1:129:B:ALA:HB1	2:290:H:TRP:HZ3	1	0.1
(1,1666)	1:129:B:ALA:HB2	2:290:H:TRP:HZ3	1	0.1
(1,1666)	1:129:B:ALA:HB3	2:290:H:TRP:HZ3	1	0.1
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD11	6	0.1
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD12	6	0.1
(1,1664)	1:137:B:PHE:HZ	2:280:H:LEU:HD13	6	0.1
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE1	18	0.1
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE2	18	0.1
(1,1655)	1:137:B:PHE:HD1	2:286:H:MET:HE3	18	0.1
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE1	18	0.1
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE2	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1655)	1:137:B:PHE:HD2	2:286:H:MET:HE3	18	0.1
(1,1641)	1:42:D:LEU:HD11	2:291:G:LEU:HD11	17	0.1
(1,1641)	1:42:D:LEU:HD11	2:291:G:LEU:HD12	17	0.1
(1,1641)	1:42:D:LEU:HD11	2:291:G:LEU:HD13	17	0.1
(1,1641)	1:42:D:LEU:HD12	2:291:G:LEU:HD11	17	0.1
(1,1641)	1:42:D:LEU:HD12	2:291:G:LEU:HD12	17	0.1
(1,1641)	1:42:D:LEU:HD12	2:291:G:LEU:HD13	17	0.1
(1,1641)	1:42:D:LEU:HD13	2:291:G:LEU:HD11	17	0.1
(1,1641)	1:42:D:LEU:HD13	2:291:G:LEU:HD12	17	0.1
(1,1641)	1:42:D:LEU:HD13	2:291:G:LEU:HD13	17	0.1
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD11	2	0.1
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD12	2	0.1
(1,1638)	1:128:D:LEU:HD11	2:291:G:LEU:HD13	2	0.1
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD11	2	0.1
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD12	2	0.1
(1,1638)	1:128:D:LEU:HD12	2:291:G:LEU:HD13	2	0.1
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD11	2	0.1
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD12	2	0.1
(1,1638)	1:128:D:LEU:HD13	2:291:G:LEU:HD13	2	0.1
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD11	17	0.1
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD12	17	0.1
(1,1626)	1:31:D:VAL:HG11	2:301:G:ILE:HD13	17	0.1
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD11	17	0.1
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD12	17	0.1
(1,1626)	1:31:D:VAL:HG12	2:301:G:ILE:HD13	17	0.1
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD11	17	0.1
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD12	17	0.1
(1,1626)	1:31:D:VAL:HG13	2:301:G:ILE:HD13	17	0.1
(1,1615)	1:40:D:VAL:HG11	2:290:G:TRP:HE1	8	0.1
(1,1615)	1:40:D:VAL:HG12	2:290:G:TRP:HE1	8	0.1
(1,1615)	1:40:D:VAL:HG13	2:290:G:TRP:HE1	8	0.1
(1,1610)	1:106:D:LEU:HD11	2:281:G:PHE:HZ	10	0.1
(1,1610)	1:106:D:LEU:HD12	2:281:G:PHE:HZ	10	0.1
(1,1610)	1:106:D:LEU:HD13	2:281:G:PHE:HZ	10	0.1
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG21	1	0.1
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG22	1	0.1
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG23	1	0.1
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG21	1	0.1
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG22	1	0.1
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG23	1	0.1
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG21	1	0.1
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG22	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG23	1	0.1
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG21	8	0.1
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG22	8	0.1
(1,1599)	1:131:B:VAL:HG21	2:309:F:THR:HG23	8	0.1
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG21	8	0.1
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG22	8	0.1
(1,1599)	1:131:B:VAL:HG22	2:309:F:THR:HG23	8	0.1
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG21	8	0.1
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG22	8	0.1
(1,1599)	1:131:B:VAL:HG23	2:309:F:THR:HG23	8	0.1
(1,1594)	1:128:C:LEU:HD11	2:290:F:TRP:HE3	17	0.1
(1,1594)	1:128:C:LEU:HD12	2:290:F:TRP:HE3	17	0.1
(1,1594)	1:128:C:LEU:HD13	2:290:F:TRP:HE3	17	0.1
(1,1594)	1:128:C:LEU:HD21	2:290:F:TRP:HE3	17	0.1
(1,1594)	1:128:C:LEU:HD22	2:290:F:TRP:HE3	17	0.1
(1,1594)	1:128:C:LEU:HD23	2:290:F:TRP:HE3	17	0.1
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD11	11	0.1
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD12	11	0.1
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD13	11	0.1
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD21	11	0.1
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD22	11	0.1
(1,1582)	1:98:C:LEU:HD11	2:280:F:LEU:HD23	11	0.1
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD11	11	0.1
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD12	11	0.1
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD13	11	0.1
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD21	11	0.1
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD22	11	0.1
(1,1582)	1:98:C:LEU:HD12	2:280:F:LEU:HD23	11	0.1
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD11	11	0.1
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD12	11	0.1
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD13	11	0.1
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD21	11	0.1
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD22	11	0.1
(1,1582)	1:98:C:LEU:HD13	2:280:F:LEU:HD23	11	0.1
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD11	11	0.1
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD12	11	0.1
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD13	11	0.1
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD21	11	0.1
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD22	11	0.1
(1,1582)	1:98:C:LEU:HD21	2:280:F:LEU:HD23	11	0.1
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD11	11	0.1
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD12	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD13	11	0.1
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD21	11	0.1
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD22	11	0.1
(1,1582)	1:98:C:LEU:HD22	2:280:F:LEU:HD23	11	0.1
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD11	11	0.1
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD12	11	0.1
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD13	11	0.1
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD21	11	0.1
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD22	11	0.1
(1,1582)	1:98:C:LEU:HD23	2:280:F:LEU:HD23	11	0.1
(1,1576)	1:89:C:ILE:HD11	2:277:F:LEU:HD11	3	0.1
(1,1576)	1:89:C:ILE:HD11	2:277:F:LEU:HD12	3	0.1
(1,1576)	1:89:C:ILE:HD11	2:277:F:LEU:HD13	3	0.1
(1,1576)	1:89:C:ILE:HD11	2:277:F:LEU:HD21	3	0.1
(1,1576)	1:89:C:ILE:HD11	2:277:F:LEU:HD22	3	0.1
(1,1576)	1:89:C:ILE:HD11	2:277:F:LEU:HD23	3	0.1
(1,1576)	1:89:C:ILE:HD12	2:277:F:LEU:HD11	3	0.1
(1,1576)	1:89:C:ILE:HD12	2:277:F:LEU:HD12	3	0.1
(1,1576)	1:89:C:ILE:HD12	2:277:F:LEU:HD13	3	0.1
(1,1576)	1:89:C:ILE:HD12	2:277:F:LEU:HD21	3	0.1
(1,1576)	1:89:C:ILE:HD12	2:277:F:LEU:HD22	3	0.1
(1,1576)	1:89:C:ILE:HD12	2:277:F:LEU:HD23	3	0.1
(1,1576)	1:89:C:ILE:HD13	2:277:F:LEU:HD11	3	0.1
(1,1576)	1:89:C:ILE:HD13	2:277:F:LEU:HD12	3	0.1
(1,1576)	1:89:C:ILE:HD13	2:277:F:LEU:HD13	3	0.1
(1,1576)	1:89:C:ILE:HD13	2:277:F:LEU:HD21	3	0.1
(1,1576)	1:89:C:ILE:HD13	2:277:F:LEU:HD22	3	0.1
(1,1576)	1:89:C:ILE:HD13	2:277:F:LEU:HD23	3	0.1
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD11	16	0.1
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD12	16	0.1
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD13	16	0.1
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD21	16	0.1
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD22	16	0.1
(1,1575)	1:87:C:ALA:HB1	2:277:F:LEU:HD23	16	0.1
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD11	16	0.1
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD12	16	0.1
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD13	16	0.1
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD21	16	0.1
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD22	16	0.1
(1,1575)	1:87:C:ALA:HB2	2:277:F:LEU:HD23	16	0.1
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD11	16	0.1
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD12	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD13	16	0.1
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD21	16	0.1
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD22	16	0.1
(1,1575)	1:87:C:ALA:HB3	2:277:F:LEU:HD23	16	0.1
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD1	5	0.1
(1,1565)	1:68:C:LEU:HD21	2:297:F:TYR:HD2	5	0.1
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD1	5	0.1
(1,1565)	1:68:C:LEU:HD22	2:297:F:TYR:HD2	5	0.1
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD1	5	0.1
(1,1565)	1:68:C:LEU:HD23	2:297:F:TYR:HD2	5	0.1
(1,1550)	1:44:C:LEU:HD21	2:286:F:MET:HE1	5	0.1
(1,1550)	1:44:C:LEU:HD21	2:286:F:MET:HE2	5	0.1
(1,1550)	1:44:C:LEU:HD21	2:286:F:MET:HE3	5	0.1
(1,1550)	1:44:C:LEU:HD22	2:286:F:MET:HE1	5	0.1
(1,1550)	1:44:C:LEU:HD22	2:286:F:MET:HE2	5	0.1
(1,1550)	1:44:C:LEU:HD22	2:286:F:MET:HE3	5	0.1
(1,1550)	1:44:C:LEU:HD23	2:286:F:MET:HE1	5	0.1
(1,1550)	1:44:C:LEU:HD23	2:286:F:MET:HE2	5	0.1
(1,1550)	1:44:C:LEU:HD23	2:286:F:MET:HE3	5	0.1
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD11	3	0.1
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD12	3	0.1
(1,1532)	1:128:A:LEU:HD11	2:291:E:LEU:HD13	3	0.1
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD11	3	0.1
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD12	3	0.1
(1,1532)	1:128:A:LEU:HD12	2:291:E:LEU:HD13	3	0.1
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD11	3	0.1
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD12	3	0.1
(1,1532)	1:128:A:LEU:HD13	2:291:E:LEU:HD13	3	0.1
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD11	3	0.1
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD12	3	0.1
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD13	3	0.1
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD21	3	0.1
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD22	3	0.1
(1,1522)	1:87:A:ALA:HB1	2:277:E:LEU:HD23	3	0.1
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD11	3	0.1
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD12	3	0.1
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD13	3	0.1
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD21	3	0.1
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD22	3	0.1
(1,1522)	1:87:A:ALA:HB2	2:277:E:LEU:HD23	3	0.1
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD11	3	0.1
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD12	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD13	3	0.1
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD21	3	0.1
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD22	3	0.1
(1,1522)	1:87:A:ALA:HB3	2:277:E:LEU:HD23	3	0.1
(1,1510)	1:74:A:PHE:HZ	2:296:E:THR:HG21	6	0.1
(1,1510)	1:74:A:PHE:HZ	2:296:E:THR:HG22	6	0.1
(1,1510)	1:74:A:PHE:HZ	2:296:E:THR:HG23	6	0.1
(1,1504)	1:106:A:LEU:HD11	2:281:E:PHE:HZ	12	0.1
(1,1504)	1:106:A:LEU:HD12	2:281:E:PHE:HZ	12	0.1
(1,1504)	1:106:A:LEU:HD13	2:281:E:PHE:HZ	12	0.1
(1,1462)	1:128:D:LEU:HD11	1:129:D:ALA:H	10	0.1
(1,1462)	1:128:D:LEU:HD12	1:129:D:ALA:H	10	0.1
(1,1462)	1:128:D:LEU:HD13	1:129:D:ALA:H	10	0.1
(1,1412)	1:99:D:GLY:H	1:102:D:CYS:H	13	0.1
(1,1412)	1:99:D:GLY:H	1:102:D:CYS:H	19	0.1
(1,1384)	1:92:D:THR:H	1:94:D:MET:H	3	0.1
(1,1383)	1:92:D:THR:H	1:93:D:GLN:H	3	0.1
(1,1362)	1:79:D:GLN:H	1:80:D:GLN:H	17	0.1
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD21	14	0.1
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD22	14	0.1
(1,1345)	1:74:D:PHE:H	1:75:D:LEU:HD23	14	0.1
(1,1338)	1:73:D:ALA:H	1:74:D:PHE:H	3	0.1
(1,1338)	1:73:D:ALA:H	1:74:D:PHE:H	12	0.1
(1,1304)	1:64:D:VAL:H	1:65:D:THR:H	16	0.1
(1,1200)	1:32:D:PHE:H	1:34:D:LYS:H	17	0.1
(1,1195)	1:31:D:VAL:HG11	1:123:D:PHE:HE1	18	0.1
(1,1195)	1:31:D:VAL:HG11	1:123:D:PHE:HE2	18	0.1
(1,1195)	1:31:D:VAL:HG12	1:123:D:PHE:HE1	18	0.1
(1,1195)	1:31:D:VAL:HG12	1:123:D:PHE:HE2	18	0.1
(1,1195)	1:31:D:VAL:HG13	1:123:D:PHE:HE1	18	0.1
(1,1195)	1:31:D:VAL:HG13	1:123:D:PHE:HE2	18	0.1
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD11	13	0.1
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD12	13	0.1
(1,1192)	1:31:D:VAL:HG11	1:68:D:LEU:HD13	13	0.1
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD11	13	0.1
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD12	13	0.1
(1,1192)	1:31:D:VAL:HG12	1:68:D:LEU:HD13	13	0.1
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD11	13	0.1
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD12	13	0.1
(1,1192)	1:31:D:VAL:HG13	1:68:D:LEU:HD13	13	0.1
(1,1185)	1:30:D:HIS:H	1:31:D:VAL:H	14	0.1
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB1	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB2	12	0.1
(1,1179)	1:25:D:ALA:HB1	1:28:D:ALA:HB3	12	0.1
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB1	12	0.1
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB2	12	0.1
(1,1179)	1:25:D:ALA:HB2	1:28:D:ALA:HB3	12	0.1
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB1	12	0.1
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB2	12	0.1
(1,1179)	1:25:D:ALA:HB3	1:28:D:ALA:HB3	12	0.1
(1,1090)	1:119:C:SER:H	1:123:C:PHE:H	1	0.1
(1,1050)	1:99:C:GLY:H	1:102:C:CYS:H	19	0.1
(1,1046)	1:98:C:LEU:HD11	1:99:C:GLY:H	19	0.1
(1,1046)	1:98:C:LEU:HD12	1:99:C:GLY:H	19	0.1
(1,1046)	1:98:C:LEU:HD13	1:99:C:GLY:H	19	0.1
(1,1045)	1:98:C:LEU:H	1:102:C:CYS:H	17	0.1
(1,1042)	1:98:C:LEU:H	1:99:C:GLY:H	6	0.1
(1,1041)	1:97:C:CYS:H	1:101:C:TYR:H	8	0.1
(1,1028)	1:93:C:GLN:H	1:96:C:HIS:H	19	0.1
(1,1023)	1:92:C:THR:H	1:93:C:GLN:H	11	0.1
(1,980)	1:73:C:ALA:H	1:74:C:PHE:H	6	0.1
(1,954)	1:64:C:VAL:H	1:76:C:CYS:H	8	0.1
(1,944)	1:62:C:VAL:H	1:78:C:VAL:H	1	0.1
(1,943)	1:62:C:VAL:H	1:63:C:THR:H	2	0.1
(1,932)	1:59:C:VAL:H	1:60:C:LEU:H	14	0.1
(1,909)	1:55:C:VAL:H	1:86:C:ILE:H	7	0.1
(1,908)	1:55:C:VAL:H	1:56:C:TYR:H	2	0.1
(1,811)	1:25:C:ALA:H	1:21:D:ILE:H	18	0.1
(1,774)	1:17:C:TYR:H	1:82:C:GLY:H	6	0.1
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE1	5	0.1
(1,741)	1:136:B:LEU:HD21	1:137:B:PHE:HE2	5	0.1
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE1	5	0.1
(1,741)	1:136:B:LEU:HD22	1:137:B:PHE:HE2	5	0.1
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE1	5	0.1
(1,741)	1:136:B:LEU:HD23	1:137:B:PHE:HE2	5	0.1
(1,732)	1:134:B:ASP:H	1:136:B:LEU:H	11	0.1
(1,713)	1:121:B:GLY:H	1:123:B:PHE:H	17	0.1
(1,696)	1:115:B:THR:H	1:116:B:SER:H	14	0.1
(1,691)	1:113:B:CYS:H	1:115:B:THR:H	15	0.1
(1,682)	1:110:B:ALA:H	1:112:B:GLU:H	18	0.1
(1,681)	1:110:B:ALA:H	1:111:B:ARG:H	4	0.1
(1,673)	1:100:B:ALA:HB1	1:133:B:PHE:H	1	0.1
(1,673)	1:100:B:ALA:HB2	1:133:B:PHE:H	1	0.1
(1,673)	1:100:B:ALA:HB3	1:133:B:PHE:H	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:100:B:ALA:H	1:102:B:CYS:H	6	0.1
(1,666)	1:99:B:GLY:H	1:100:B:ALA:H	11	0.1
(1,665)	1:98:B:LEU:HD11	1:99:B:GLY:H	5	0.1
(1,665)	1:98:B:LEU:HD12	1:99:B:GLY:H	5	0.1
(1,665)	1:98:B:LEU:HD13	1:99:B:GLY:H	5	0.1
(1,646)	1:94:B:MET:H	1:96:B:HIS:H	19	0.1
(1,641)	1:92:B:THR:H	1:95:B:ALA:H	19	0.1
(1,639)	1:92:B:THR:H	1:93:B:GLN:H	20	0.1
(1,553)	1:58:B:VAL:HG11	1:59:B:VAL:H	17	0.1
(1,553)	1:58:B:VAL:HG12	1:59:B:VAL:H	17	0.1
(1,553)	1:58:B:VAL:HG13	1:59:B:VAL:H	17	0.1
(1,504)	1:45:B:ASP:H	1:61:B:ARG:H	4	0.1
(1,499)	1:44:B:LEU:HD11	1:45:B:ASP:H	14	0.1
(1,499)	1:44:B:LEU:HD12	1:45:B:ASP:H	14	0.1
(1,499)	1:44:B:LEU:HD13	1:45:B:ASP:H	14	0.1
(1,498)	1:44:B:LEU:H	1:63:B:THR:H	1	0.1
(1,493)	1:43:B:ASP:H	1:44:B:LEU:H	7	0.1
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	7	0.1
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	7	0.1
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	7	0.1
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	7	0.1
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	7	0.1
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	7	0.1
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	7	0.1
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	7	0.1
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	7	0.1
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	19	0.1
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	19	0.1
(1,449)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	19	0.1
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	19	0.1
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	19	0.1
(1,449)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	19	0.1
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	19	0.1
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	19	0.1
(1,449)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	19	0.1
(1,438)	1:22:B:SER:H	1:77:B:GLU:H	11	0.1
(1,430)	1:19:B:LYS:H	1:79:B:GLN:H	10	0.1
(1,417)	1:14:B:GLN:H	1:15:B:ARG:H	7	0.1
(1,395)	1:138:A:MET:H	1:140:A:TYR:H	8	0.1
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	16	0.1
(1,377)	1:133:A:PHE:H	1:135:A:ALA:H	18	0.1
(1,362)	1:126:A:LEU:H	1:127:A:ASN:H	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:122:A:THR:H	1:18:B:THR:H	2	0.1
(1,332)	1:112:A:GLU:H	1:113:A:CYS:H	8	0.1
(1,319)	1:101:A:TYR:H	1:102:A:CYS:H	7	0.1
(1,285)	1:92:A:THR:H	1:94:A:MET:H	6	0.1
(1,263)	1:79:A:GLN:H	1:80:A:GLN:H	10	0.1
(1,236)	1:69:A:GLY:H	1:71:A:GLU:H	14	0.1
(1,232)	1:68:A:LEU:H	1:73:A:ALA:H	3	0.1
(1,171)	1:56:A:TYR:H	1:86:A:ILE:H	20	0.1
(1,163)	1:54:A:ASP:H	1:55:A:VAL:H	5	0.1
(1,163)	1:54:A:ASP:H	1:55:A:VAL:H	9	0.1
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG11	20	0.1
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG12	20	0.1
(1,102)	1:40:A:VAL:HG11	1:64:A:VAL:HG13	20	0.1
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG11	20	0.1
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG12	20	0.1
(1,102)	1:40:A:VAL:HG12	1:64:A:VAL:HG13	20	0.1
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG11	20	0.1
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG12	20	0.1
(1,102)	1:40:A:VAL:HG13	1:64:A:VAL:HG13	20	0.1
(1,50)	1:23:A:PHE:H	1:21:B:ILE:H	15	0.1
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	11	0.1
(1,40)	1:21:A:ILE:H	1:22:A:SER:H	16	0.1
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB1	13	0.1
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB2	13	0.1
(1,27)	1:17:A:TYR:HE1	1:28:B:ALA:HB3	13	0.1
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB1	13	0.1
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB2	13	0.1
(1,27)	1:17:A:TYR:HE2	1:28:B:ALA:HB3	13	0.1
(1,21)	1:15:A:ARG:H	1:83:A:ILE:H	5	0.1

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

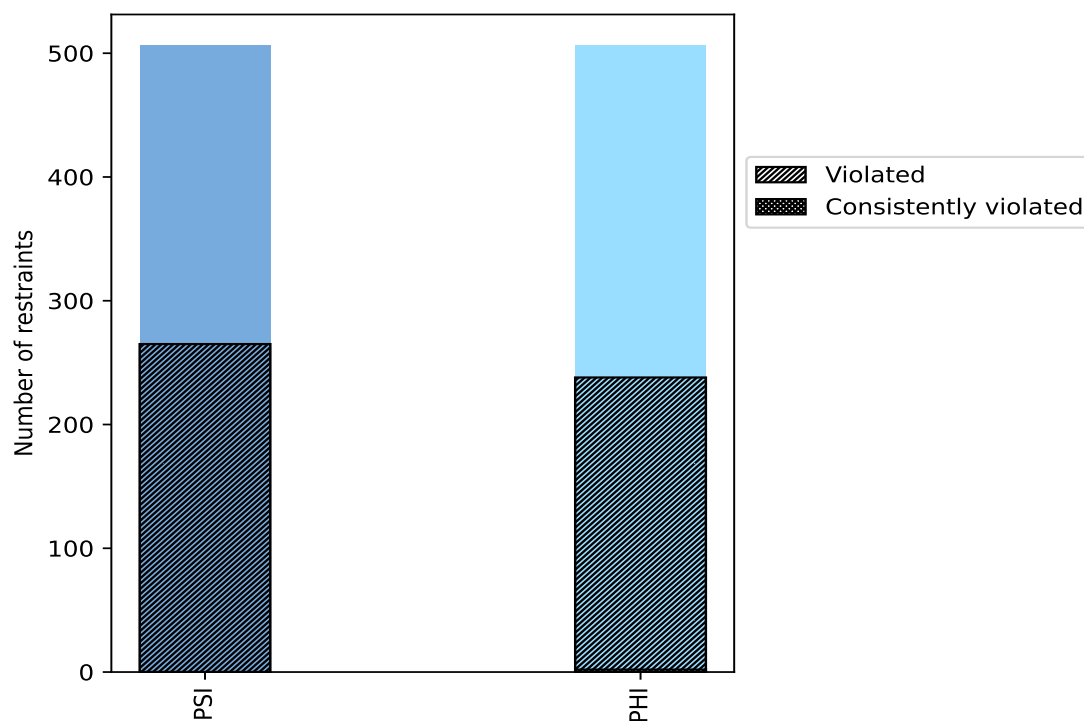
### 10.1 Summary of dihedral-angle violations [i](#)

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	506	50.0	265	52.4	26.2	0	0.0	0.0
PHI	506	50.0	238	47.0	23.5	2	0.4	0.2
Total	1012	100.0	503	49.7	49.7	2	0.2	0.2

<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](#)



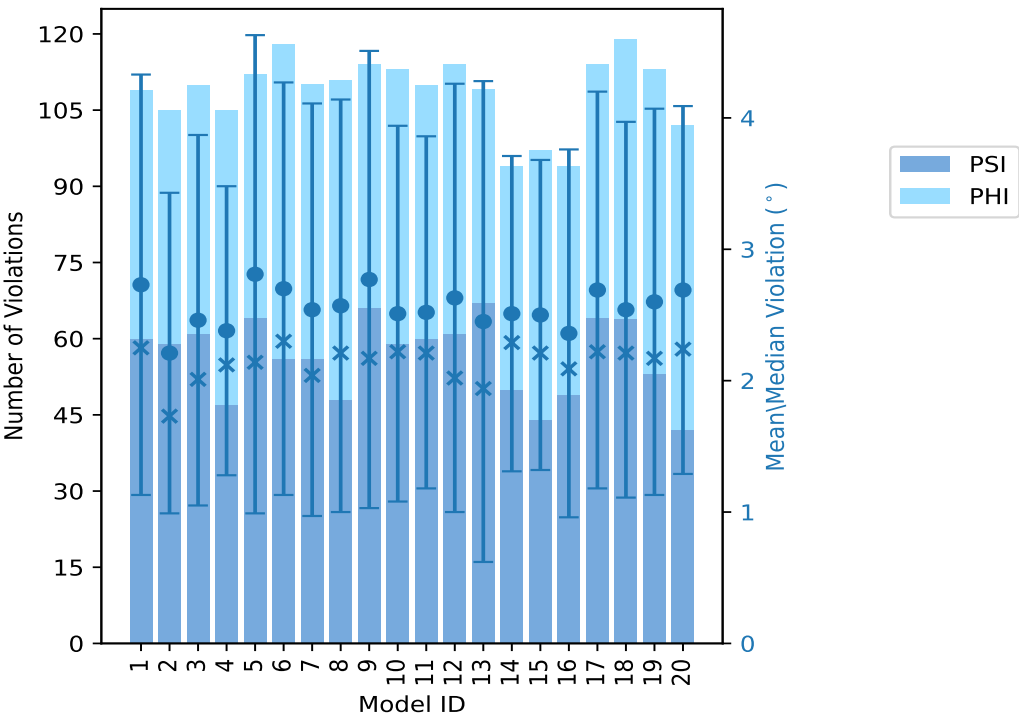
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	60	49	109	2.73	10.34	1.6	2.25
2	59	46	105	2.21	7.93	1.22	1.73
3	61	49	110	2.46	9.86	1.41	2.01
4	47	58	105	2.38	6.32	1.1	2.12
5	64	48	112	2.81	10.4	1.82	2.14
6	56	62	118	2.7	11.0	1.57	2.3
7	56	54	110	2.54	8.54	1.57	2.04
8	48	63	111	2.57	8.9	1.57	2.21
9	66	48	114	2.77	11.97	1.74	2.17
10	59	54	113	2.51	8.93	1.43	2.22
11	60	50	110	2.52	9.81	1.34	2.21
12	61	53	114	2.63	10.08	1.63	2.02
13	67	42	109	2.45	11.73	1.83	1.94
14	50	44	94	2.51	5.99	1.2	2.29
15	44	53	97	2.5	6.29	1.18	2.21
16	49	45	94	2.36	8.44	1.4	2.09
17	64	50	114	2.69	8.74	1.51	2.22
18	64	55	119	2.54	8.4	1.43	2.21
19	53	60	113	2.6	9.58	1.47	2.17
20	42	60	102	2.69	8.11	1.4	2.24

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>	%
77	56	133	1	5.0
40	57	97	2	10.0
35	30	65	3	15.0
24	22	46	4	20.0
12	12	24	5	25.0
19	10	29	6	30.0
13	7	20	7	35.0
8	5	13	8	40.0
7	6	13	9	45.0
5	5	10	10	50.0
6	4	10	11	55.0

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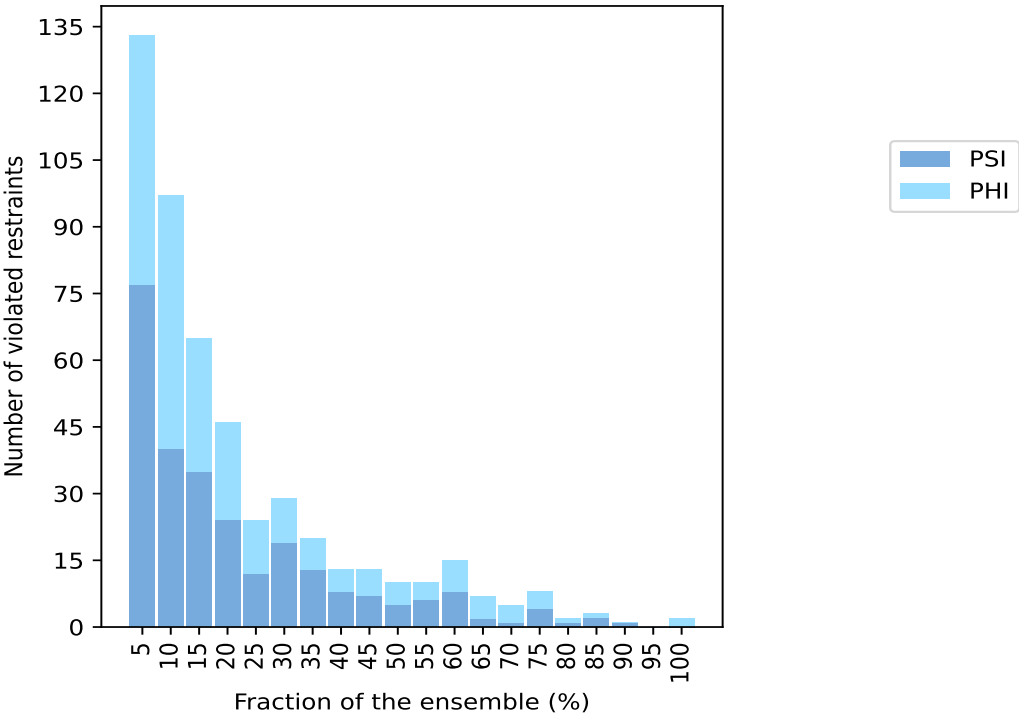


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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
8	7	15	12	60.0
2	5	7	13	65.0
1	4	5	14	70.0
4	4	8	15	75.0
1	1	2	16	80.0
2	1	3	17	85.0
1	0	1	18	90.0
0	0	0	19	95.0
0	2	2	20	100.0

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

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

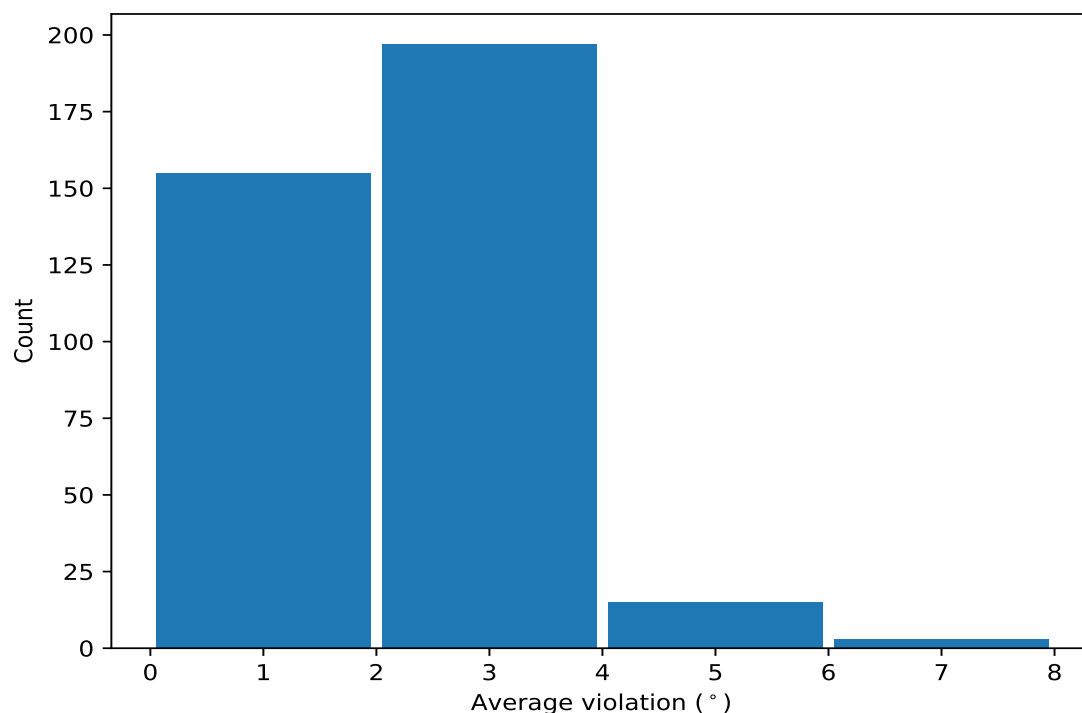


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	20	6.86	2.33	7.76
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	20	3.06	1.28	2.86
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	18	3.77	1.33	3.7
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	17	4.88	1.83	5.15
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	17	3.62	2.06	3.28
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	17	2.26	0.83	2.24
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	16	6.33	2.68	5.98
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	16	2.32	0.92	1.88
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	15	4.67	2.1	4.36
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	15	3.76	1.61	3.36
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	15	3.75	2.16	3.28
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	15	3.09	1.36	3.2
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	15	2.66	1.53	2.03
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	15	2.63	0.79	2.65
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	15	2.55	1.06	2.42
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	15	2.3	1.12	1.83
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	14	4.48	1.9	4.94
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	14	4.01	3.16	2.91
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	14	2.98	1.8	2.36
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	14	2.92	1.06	2.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	14	2.12	0.65	1.86
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	13	3.7	1.18	3.41
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	13	2.98	1.19	2.78
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	13	2.72	1.38	2.36
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	13	2.59	1.0	2.49
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	13	2.42	0.76	2.49
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	13	2.17	0.5	2.21
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	13	1.9	0.65	1.66
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	12	6.14	3.07	6.62
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	12	4.17	1.8	3.9
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	12	3.34	1.69	2.84
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	12	3.04	1.22	3.34
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	12	2.87	1.17	2.93
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	12	2.69	0.72	2.76
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	12	2.66	0.67	2.7
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	12	2.55	1.02	2.26
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	12	2.5	0.95	2.29
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	12	2.33	0.98	2.1
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	12	2.31	0.79	2.47
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	12	2.28	1.19	1.96
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	12	2.07	0.68	1.96
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	12	1.84	0.49	1.71
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	12	1.8	0.55	1.68
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	11	3.62	2.43	2.82
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	11	3.52	1.16	3.53
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	11	3.3	1.11	2.97
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	11	3.15	1.23	3.15
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	11	3.09	1.1	3.26
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	11	2.97	1.43	2.53
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	11	2.59	0.78	2.65
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	11	2.58	0.79	2.39
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	11	1.84	0.6	1.92
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	11	1.51	0.31	1.55
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	10	4.89	0.99	5.14
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	10	4.62	1.57	4.59
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	10	3.0	1.48	3.16
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	10	2.82	1.41	2.69
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	10	2.82	1.33	2.54
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	10	2.64	1.11	2.71
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	10	2.62	0.87	2.74
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	10	2.39	1.23	2.04
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	10	2.21	0.87	2.04
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	10	1.71	0.64	1.55
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	9	4.13	1.38	4.36
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	9	4.0	1.61	4.19
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	9	3.32	1.38	3.27
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	9	3.24	1.52	3.08
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	9	2.7	1.24	2.5
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	9	2.41	0.96	2.18
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	9	2.39	0.28	2.41
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	9	2.38	0.97	2.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	9	2.29	0.79	1.87
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	9	2.09	1.04	1.65
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	9	1.97	0.9	1.55
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	9	1.83	0.58	1.74
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	9	1.67	0.43	1.48
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	8	3.24	1.12	3.32
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	8	2.86	0.59	2.98
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	8	2.6	1.39	2.52
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	8	2.52	1.0	2.36
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	8	2.36	1.06	2.0
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	8	2.27	0.73	1.96
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	8	2.11	0.91	1.82
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	8	2.0	0.76	1.92
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	8	1.95	0.96	1.6
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	8	1.78	0.75	1.48
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	8	1.76	0.69	1.43
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	8	1.75	0.39	1.89
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	8	1.58	0.41	1.75
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	7	3.99	1.67	4.31
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	7	3.49	2.97	1.73
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	7	3.26	0.6	3.14
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	7	3.23	1.12	3.14
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	7	2.84	2.12	1.66
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	7	2.83	1.77	1.86
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	7	2.72	1.12	2.94
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	7	2.61	1.1	2.3
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	7	2.55	1.11	1.98
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	7	2.48	0.92	2.51
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	7	2.4	1.3	1.7
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	7	2.4	0.52	2.43
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	7	2.35	0.76	2.44
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	7	2.31	0.99	2.61
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	7	2.25	1.21	1.66
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	7	2.16	0.58	2.08
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	7	2.12	1.05	1.77
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	7	1.86	0.46	1.89
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	7	1.84	0.73	1.78
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	7	1.63	0.33	1.62
(1,808)	1:36:D:TRP:C	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	6	3.68	1.96	3.18
(1,767)	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	1:15:D:ARG:N	6	3.59	0.84	3.7
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	6	3.2	0.73	3.46
(1,375)	1:72:B:THR:N	1:72:B:THR:CA	1:72:B:THR:C	1:73:B:ALA:N	6	3.19	1.21	2.68
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	6	2.77	1.56	2.39
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	6	2.63	1.67	1.89
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	6	2.57	1.06	2.4
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	6	2.47	0.62	2.33
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	6	2.46	1.19	2.14
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	6	2.43	0.95	2.23
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	6	2.42	1.05	2.35
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	6	2.42	0.58	2.3
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	6	2.4	0.35	2.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	6	2.39	0.44	2.41
(1,542)	1:27:C:ASN:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	6	2.27	0.51	2.12
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	6	2.2	0.77	1.96
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	6	2.16	0.45	2.05
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	6	2.13	0.5	2.28
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	6	2.12	1.21	1.33
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	6	1.91	0.79	1.64
(1,352)	1:60:B:LEU:C	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	6	1.84	0.62	1.66
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	6	1.8	0.42	1.66
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	6	1.71	0.38	1.66
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	6	1.66	0.43	1.44
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	6	1.64	0.39	1.62
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	6	1.63	0.95	1.22
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	6	1.57	0.33	1.62
(1,472)	1:122:B:THR:C	1:123:B:PHE:N	1:123:B:PHE:CA	1:123:B:PHE:C	6	1.28	0.22	1.27
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	6	1.21	0.12	1.22
(1,557)	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	1:37:C:GLN:N	5	5.07	2.98	5.68
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	5	3.3	1.16	3.51
(1,76)	1:49:A:SER:C	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	5	3.21	1.37	3.02
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	5	2.71	0.79	2.94
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	5	2.71	0.56	2.7
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	5	2.71	1.02	2.45
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	5	2.69	1.15	2.19
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	5	2.61	1.34	1.64
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	5	2.59	0.91	2.89
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	5	2.5	0.68	2.33
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	5	2.47	0.74	2.58
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	5	2.2	0.85	2.63
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	5	2.01	1.01	1.43
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	5	2.01	0.8	1.87
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	5	1.88	0.73	1.68
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	5	1.85	0.75	1.56
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	5	1.83	0.61	1.55
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	5	1.76	0.45	1.87
(1,290)	1:27:B:ASN:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	5	1.76	0.53	2.02
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	5	1.71	0.26	1.82
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	5	1.57	0.21	1.61
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	5	1.54	0.43	1.51
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	5	1.49	0.5	1.33
(1,128)	1:75:A:LEU:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	5	1.31	0.14	1.24
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	4	4.44	1.67	4.62
(1,299)	1:33:B:GLN:N	1:33:B:GLN:CA	1:33:B:GLN:C	1:34:B:LYS:N	4	4.41	1.97	4.35
(1,999)	1:137:D:PHE:N	1:137:D:PHE:CA	1:137:D:PHE:C	1:138:D:MET:N	4	3.81	2.11	3.76
(1,302)	1:34:B:LYS:C	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	4	3.53	0.92	3.47
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	4	3.06	0.4	2.93
(1,784)	1:22:D:SER:C	1:23:D:PHE:N	1:23:D:PHE:CA	1:23:D:PHE:C	4	2.78	0.88	2.96
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	4	2.62	1.44	2.35
(1,830)	1:48:D:SER:C	1:49:D:SER:N	1:49:D:SER:CA	1:49:D:SER:C	4	2.6	1.04	2.33
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	4	2.47	0.24	2.42
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	4	2.46	0.73	2.46
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	4	2.46	1.18	2.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	4	2.42	0.65	2.1
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	4	2.42	0.93	2.28
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	4	2.4	0.28	2.45
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	4	2.33	0.72	2.1
(1,105)	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1:65:A:THR:N	4	2.33	0.59	2.3
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	4	2.26	0.62	2.42
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	4	2.22	0.33	2.21
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	4	2.22	0.67	2.51
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	4	2.15	0.49	2.3
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	4	2.1	0.8	1.96
(1,599)	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	1:59:C:VAL:N	4	2.1	1.24	1.58
(1,575)	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	1:47:C:ALA:N	4	2.06	0.3	2.05
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	4	2.03	1.15	1.46
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	4	2.0	1.15	1.53
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	4	1.97	1.04	1.44
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	4	1.92	0.41	1.96
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	4	1.91	0.56	1.94
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	4	1.86	0.61	1.81
(1,400)	1:84:B:PHE:C	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	4	1.84	0.46	1.9
(1,574)	1:45:C:ASP:C	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	4	1.81	0.36	1.93
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	4	1.81	0.4	1.97
(1,581)	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	1:50:C:GLN:N	4	1.8	0.27	1.87
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	4	1.8	0.57	1.6
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	4	1.77	0.58	1.57
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	4	1.7	0.74	1.36
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	4	1.68	0.4	1.68
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	4	1.67	0.33	1.52
(1,519)	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	1:16:C:ILE:N	4	1.62	0.35	1.44
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	4	1.61	0.27	1.52
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	4	1.57	0.15	1.58
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	4	1.56	0.4	1.47
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	4	1.54	0.41	1.54
(1,214)	1:120:A:ARG:C	1:121:A:GLY:N	1:121:A:GLY:CA	1:121:A:GLY:C	4	1.46	0.17	1.51
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	4	1.39	0.31	1.28
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	4	1.34	0.19	1.34
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	3	3.32	0.7	3.09
(1,307)	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	1:38:B:PRO:N	3	3.23	2.3	2.13
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	3	2.9	0.9	3.39
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	3	2.86	1.53	2.56
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	3	2.82	0.59	3.05
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	3	2.75	0.19	2.68
(1,535)	1:23:C:PHE:N	1:23:C:PHE:CA	1:23:C:PHE:C	1:24:C:GLU:N	3	2.65	0.8	2.63
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	3	2.64	0.23	2.66
(1,367)	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	1:69:B:GLY:N	3	2.55	1.08	2.69
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	3	2.53	0.94	2.08
(1,55)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:VAL:N	3	2.48	0.75	2.14
(1,915)	1:91:D:GLY:N	1:91:D:GLY:CA	1:91:D:GLY:C	1:92:D:THR:N	3	2.47	1.13	2.52
(1,61)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:ASP:N	3	2.41	0.89	2.28
(1,152)	1:87:A:ALA:C	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	3	2.36	0.74	1.95
(1,32)	1:24:A:GLU:C	1:25:A:ALA:N	1:25:A:ALA:CA	1:25:A:ALA:C	3	2.36	0.99	2.42
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	3	2.36	1.57	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,883)	1:75:D:LEU:N	1:75:D:LEU:CA	1:75:D:LEU:C	1:76:D:CYS:N	3	2.36	0.8	2.2
(1,673)	1:95:C:ALA:N	1:95:C:ALA:CA	1:95:C:ALA:C	1:96:C:HIS:N	3	2.24	0.9	2.21
(1,264)	1:13:B:ILE:C	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	3	2.16	1.03	1.79
(1,287)	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	1:26:B:PRO:N	3	2.15	0.58	2.53
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	3	2.13	0.65	1.89
(1,797)	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	1:32:D:PHE:N	3	2.1	0.36	2.32
(1,75)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLN:N	3	2.09	0.38	1.84
(1,731)	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	1:128:C:LEU:N	3	2.07	0.53	1.93
(1,758)	1:9:D:MET:C	1:10:D:THR:N	1:10:D:THR:CA	1:10:D:THR:C	3	2.05	0.8	1.85
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	3	2.02	0.53	2.19
(1,832)	1:49:D:SER:C	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	3	2.02	0.31	2.01
(1,146)	1:84:A:PHE:C	1:85:A:SER:N	1:85:A:SER:CA	1:85:A:SER:C	3	1.96	0.79	1.73
(1,503)	1:140:B:TYR:N	1:140:B:TYR:CA	1:140:B:TYR:C	1:141:B:LEU:N	3	1.96	0.72	1.66
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	3	1.92	0.87	1.49
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	3	1.9	0.57	2.22
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	3	1.89	0.42	2.12
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	3	1.88	0.27	1.96
(1,571)	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	1:45:C:ASP:N	3	1.86	0.76	1.37
(1,800)	1:32:D:PHE:C	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	3	1.85	0.7	1.79
(1,754)	1:139:C:ASN:C	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	3	1.84	0.2	1.91
(1,787)	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	1:25:D:ALA:N	3	1.84	0.65	1.46
(1,934)	1:100:D:ALA:C	1:101:D:TYR:N	1:101:D:TYR:CA	1:101:D:TYR:C	3	1.82	0.14	1.91
(1,738)	1:131:C:VAL:C	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	3	1.8	0.54	1.83
(1,626)	1:71:C:GLU:C	1:72:C:THR:N	1:72:C:THR:CA	1:72:C:THR:C	3	1.8	0.52	1.58
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	3	1.79	0.41	2.05
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	3	1.76	0.53	1.63
(1,393)	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1:82:B:GLY:N	3	1.74	0.55	1.44
(1,635)	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1:77:C:GLU:N	3	1.73	0.5	2.07
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	3	1.7	0.27	1.72
(1,684)	1:100:C:ALA:C	1:101:C:TYR:N	1:101:C:TYR:CA	1:101:C:TYR:C	3	1.7	0.16	1.77
(1,723)	1:122:C:THR:N	1:122:C:THR:CA	1:122:C:THR:C	1:123:C:PHE:N	3	1.67	0.27	1.81
(1,106)	1:64:A:VAL:C	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	3	1.62	0.39	1.76
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	3	1.62	0.29	1.79
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	3	1.61	0.53	1.26
(1,222)	1:125:A:GLN:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	3	1.6	0.45	1.29
(1,872)	1:69:D:GLY:C	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	3	1.57	0.41	1.34
(1,647)	1:82:C:GLY:N	1:82:C:GLY:CA	1:82:C:GLY:C	1:83:C:ILE:N	3	1.54	0.26	1.48
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	3	1.53	0.27	1.66
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	3	1.52	0.22	1.47
(1,786)	1:23:D:PHE:C	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	3	1.49	0.23	1.44
(1,903)	1:85:D:SER:N	1:85:D:SER:CA	1:85:D:SER:C	1:86:D:ILE:N	3	1.46	0.04	1.48
(1,648)	1:82:C:GLY:C	1:83:C:ILE:N	1:83:C:ILE:CA	1:83:C:ILE:C	3	1.45	0.55	1.11
(1,659)	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	1:89:C:ILE:N	3	1.36	0.29	1.21
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	3	1.32	0.09	1.38
(1,481)	1:128:B:LEU:N	1:128:B:LEU:CA	1:128:B:LEU:C	1:129:B:ALA:N	3	1.31	0.07	1.3
(1,136)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	3	1.25	0.14	1.24
(1,414)	1:91:B:GLY:C	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	3	1.23	0.2	1.11
(1,173)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:GLY:N	3	1.19	0.03	1.18
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	3	1.18	0.09	1.12
(1,750)	1:137:C:PHE:C	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	2	4.75	0.21	4.75
(1,39)	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	1:31:A:VAL:N	2	4.39	2.52	4.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,977)	1:125:D:GLN:N	1:125:D:GLN:CA	1:125:D:GLN:C	1:126:D:LEU:N	2	4.03	0.07	4.03
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	2	3.74	0.38	3.74
(1,411)	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	1:91:B:GLY:N	2	3.44	1.32	3.44
(1,809)	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	1:38:D:PRO:N	2	3.33	1.75	3.33
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	2	3.18	1.2	3.18
(1,86)	1:54:A:ASP:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	2	3.14	1.05	3.14
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	2	3.03	1.91	3.03
(1,558)	1:36:C:TRP:C	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	2	3.02	0.38	3.02
(1,306)	1:36:B:TRP:C	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	2	2.94	1.69	2.94
(1,749)	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	1:138:C:MET:N	2	2.92	1.82	2.92
(1,727)	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1:126:C:LEU:N	2	2.76	0.03	2.76
(1,1006)	1:140:D:TYR:C	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	2	2.74	0.76	2.74
(1,623)	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1:71:C:GLU:N	2	2.74	0.05	2.74
(1,660)	1:88:C:GLY:C	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	2	2.7	0.36	2.7
(1,370)	1:69:B:GLY:C	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	2	2.66	1.3	2.66
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	2	2.63	0.06	2.63
(1,30)	1:23:A:PHE:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	2	2.58	0.32	2.58
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	2	2.55	0.71	2.55
(1,607)	1:62:C:VAL:N	1:62:C:VAL:CA	1:62:C:VAL:C	1:63:C:THR:N	2	2.54	0.61	2.54
(1,538)	1:24:C:GLU:C	1:25:C:ALA:N	1:25:C:ALA:CA	1:25:C:ALA:C	2	2.5	0.09	2.5
(1,28)	1:22:A:SER:C	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	2	2.49	0.73	2.49
(1,621)	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	1:70:C:GLU:N	2	2.47	0.32	2.47
(1,799)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:GLN:N	2	2.42	1.04	2.42
(1,409)	1:89:B:ILE:N	1:89:B:ILE:CA	1:89:B:ILE:C	1:90:B:GLU:N	2	2.38	0.46	2.38
(1,739)	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	1:133:C:PHE:N	2	2.34	1.3	2.34
(1,149)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:ALA:N	2	2.28	0.6	2.28
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	2	2.11	0.74	2.11
(1,119)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:THR:N	2	2.11	0.6	2.11
(1,156)	1:89:A:ILE:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	2	2.1	0.51	2.1
(1,126)	1:74:A:PHE:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	2	2.05	0.64	2.05
(1,315)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:ASP:N	2	2.05	0.34	2.05
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	2	2.04	0.06	2.04
(1,728)	1:125:C:GLN:C	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	2	2.02	0.9	2.02
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	2	2.02	0.09	2.02
(1,603)	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	1:61:C:ARG:N	2	2.02	0.59	2.02
(1,347)	1:58:B:VAL:N	1:58:B:VAL:CA	1:58:B:VAL:C	1:59:B:VAL:N	2	2.01	0.53	2.01
(1,35)	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1:28:A:ALA:N	2	1.99	0.74	1.99
(1,383)	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	1:77:B:GLU:N	2	1.98	0.96	1.98
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	2	1.96	0.08	1.96
(1,734)	1:128:C:LEU:C	1:129:C:ALA:N	1:129:C:ALA:CA	1:129:C:ALA:C	2	1.94	0.37	1.94
(1,476)	1:125:B:GLN:C	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	2	1.91	0.3	1.91
(1,912)	1:89:D:ILE:C	1:90:D:GLU:N	1:90:D:GLU:CA	1:90:D:GLU:C	2	1.9	0.13	1.9
(1,788)	1:24:D:GLU:C	1:25:D:ALA:N	1:25:D:ALA:CA	1:25:D:ALA:C	2	1.88	0.86	1.88
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	2	1.87	0.5	1.87
(1,709)	1:115:C:THR:N	1:115:C:THR:CA	1:115:C:THR:C	1:116:C:SER:N	2	1.87	0.59	1.87
(1,631)	1:74:C:PHE:N	1:74:C:PHE:CA	1:74:C:PHE:C	1:75:C:LEU:N	2	1.86	0.36	1.86
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	2	1.79	0.4	1.79
(1,556)	1:35:C:ASP:C	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	2	1.78	0.18	1.78
(1,602)	1:59:C:VAL:C	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	2	1.76	0.14	1.76
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	2	1.76	0.42	1.76
(1,783)	1:22:D:SER:N	1:22:D:SER:CA	1:22:D:SER:C	1:23:D:PHE:N	2	1.74	0.74	1.74

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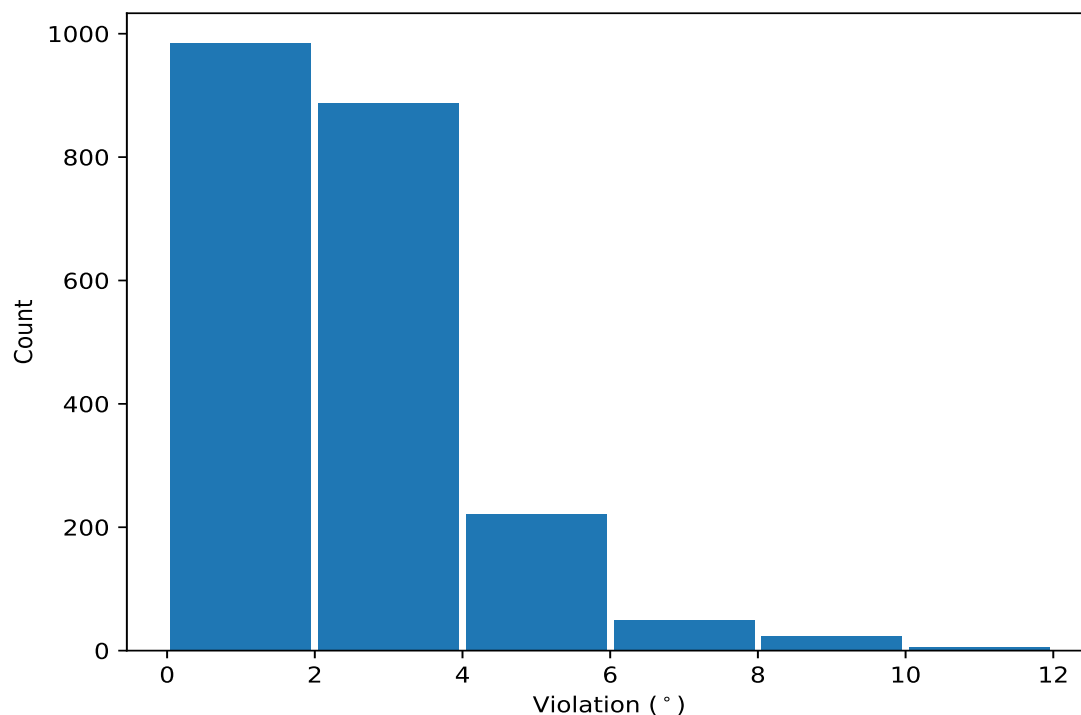
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,94)	1:58:A:VAL:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	2	1.74	0.21	1.74
(1,288)	1:26:B:PRO:C	1:27:B:ASN:N	1:27:B:ASN:CA	1:27:B:ASN:C	2	1.72	0.12	1.72
(1,552)	1:33:C:GLN:C	1:34:C:LYS:N	1:34:C:LYS:CA	1:34:C:LYS:C	2	1.72	0.3	1.72
(1,138)	1:80:A:GLN:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	2	1.72	0.04	1.72
(1,633)	1:75:C:LEU:N	1:75:C:LEU:CA	1:75:C:LEU:C	1:76:C:CYS:N	2	1.69	0.02	1.69
(1,69)	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1:47:A:ALA:N	2	1.68	0.19	1.68
(1,223)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:ASN:N	2	1.68	0.26	1.68
(1,130)	1:76:A:CYS:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	2	1.65	0.64	1.65
(1,53)	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1:38:A:PRO:N	2	1.64	0.17	1.64
(1,178)	1:100:A:ALA:C	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	2	1.64	0.18	1.64
(1,820)	1:43:D:ASP:C	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	2	1.61	0.53	1.61
(1,350)	1:59:B:VAL:C	1:60:B:LEU:N	1:60:B:LEU:CA	1:60:B:LEU:C	2	1.6	0.5	1.6
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	2	1.58	0.32	1.58
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	2	1.56	0.05	1.56
(1,612)	1:64:C:VAL:C	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	2	1.54	0.21	1.54
(1,865)	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	1:67:D:SER:N	2	1.54	0.13	1.54
(1,976)	1:124:D:PRO:C	1:125:D:GLN:N	1:125:D:GLN:CA	1:125:D:GLN:C	2	1.54	0.4	1.54
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	2	1.54	0.17	1.54
(1,272)	1:17:B:TYR:C	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	2	1.5	0.45	1.5
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	2	1.5	0.03	1.5
(1,504)	1:140:B:TYR:C	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	2	1.48	0.18	1.48
(1,263)	1:13:B:ILE:N	1:13:B:ILE:CA	1:13:B:ILE:C	1:14:B:GLN:N	2	1.44	0.11	1.44
(1,516)	1:13:C:ILE:C	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	2	1.42	0.31	1.42
(1,671)	1:94:C:MET:N	1:94:C:MET:CA	1:94:C:MET:C	1:95:C:ALA:N	2	1.42	0.11	1.42
(1,274)	1:18:B:THR:C	1:19:B:LYS:N	1:19:B:LYS:CA	1:19:B:LYS:C	2	1.42	0.04	1.42
(1,848)	1:57:D:GLU:C	1:58:D:VAL:N	1:58:D:VAL:CA	1:58:D:VAL:C	2	1.42	0.2	1.42
(1,29)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	2	1.34	0.32	1.34
(1,822)	1:44:D:LEU:C	1:45:D:ASP:N	1:45:D:ASP:CA	1:45:D:ASP:C	2	1.34	0.22	1.34
(1,679)	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	1:99:C:GLY:N	2	1.34	0.16	1.34
(1,835)	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	1:52:D:ALA:N	2	1.32	0.31	1.32
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	2	1.32	0.02	1.32
(1,348)	1:58:B:VAL:C	1:59:B:VAL:N	1:59:B:VAL:CA	1:59:B:VAL:C	2	1.28	0.24	1.28
(1,403)	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1:87:B:ALA:N	2	1.28	0.17	1.28
(1,303)	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	1:36:B:TRP:N	2	1.28	0.16	1.28
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	2	1.27	0.09	1.27
(1,1012)	1:143:D:GLN:C	1:144:D:GLN:N	1:144:D:GLN:CA	1:144:D:GLN:C	2	1.27	0.01	1.27
(1,140)	1:81:A:GLY:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	2	1.23	0.07	1.23
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	2	1.2	0.1	1.2
(1,34)	1:26:A:PRO:C	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	2	1.16	0.1	1.16
(1,510)	1:10:C:THR:C	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	2	1.12	0.09	1.12
(1,616)	1:66:C:ALA:C	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	2	1.09	0.0	1.09
(1,606)	1:61:C:ARG:C	1:62:C:VAL:N	1:62:C:VAL:CA	1:62:C:VAL:C	2	1.09	0.07	1.09
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	2	1.08	0.06	1.08
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	2	1.04	0.02	1.04

<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 (°)
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	9	11.97
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	13	11.73
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	6	11.0
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	5	10.4
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1	10.34
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	12	10.08
(1,557)	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	1:37:C:GLN:N	3	9.86
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	11	9.81
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	13	9.68
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	19	9.58
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	13	9.55
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	9	9.21
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1	9.04
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	5	8.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	10	8.93
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	8	8.9
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	8	8.87
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	6	8.81
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	17	8.74
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	8	8.56
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	7	8.54
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	5	8.53
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	16	8.44
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	18	8.4
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	12	8.39
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	12	8.3
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	5	8.28
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	7	8.16
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	20	8.11
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	2	7.93
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	9	7.82
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	16	7.76
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	13	7.75
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	3	7.72
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	20	7.5
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	18	7.43
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	17	7.2
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	19	7.15
(1,299)	1:33:B:GLN:N	1:33:B:GLN:CA	1:33:B:GLN:C	1:34:B:LYS:N	13	7.15
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	20	7.07
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	7	6.95
(1,39)	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	1:31:A:VAL:N	5	6.91
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1	6.83
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	7	6.77
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	12	6.71
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	16	6.62
(1,808)	1:36:D:TRP:C	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	12	6.6
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	1	6.58
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	8	6.56
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	9	6.5
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	9	6.46
(1,307)	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	1:38:B:PRO:N	19	6.43
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	6	6.39
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	6	6.38
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	10	6.36
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	8	6.35
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	5	6.34
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	20	6.34
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	8	6.33
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	18	6.33
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	4	6.32
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	3	6.29
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	15	6.29
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	7	6.29
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	15	6.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	18	6.22
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	18	6.22
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	17	6.18
(1,999)	1:137:D:PHE:N	1:137:D:PHE:CA	1:137:D:PHE:C	1:138:D:MET:N	1	6.14
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	10	6.14
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	5	6.11
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	7	6.08
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	9	6.08
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	8	6.08
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	5	6.05
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	2	6.03
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	19	6.02
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	20	6.01
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1	6.01
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	14	5.99
(1,557)	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	1:37:C:GLN:N	11	5.99
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	10	5.98
(1,808)	1:36:D:TRP:C	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	16	5.93
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	11	5.92
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	11	5.92
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	6	5.88
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	6	5.88
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	17	5.83
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	5	5.78
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	1	5.78
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	13	5.75
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	17	5.73
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	6	5.72
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	12	5.71
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	17	5.71
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	14	5.7
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	17	5.69
(1,999)	1:137:D:PHE:N	1:137:D:PHE:CA	1:137:D:PHE:C	1:138:D:MET:N	10	5.68
(1,557)	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	1:37:C:GLN:N	15	5.68
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	13	5.68
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	9	5.68
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	2	5.66
(1,76)	1:49:A:SER:C	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	5	5.66
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	17	5.65
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	4	5.65
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	13	5.61
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	4	5.59
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	6	5.59
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	9	5.55
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	5	5.55
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	19	5.54
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	10	5.53
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	9	5.51
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	17	5.51
(1,819)	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	1:44:D:LEU:N	19	5.47
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	10	5.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	20	5.37
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	6	5.33
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	17	5.32
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	2	5.31
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	14	5.31
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	6	5.3
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	5	5.3
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	19	5.3
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	18	5.28
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	14	5.24
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	1	5.23
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	19	5.21
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	10	5.19
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	19	5.18
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	7	5.18
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	9	5.16
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	12	5.15
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	17	5.15
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	19	5.15
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	19	5.13
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	4	5.13
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	7	5.11
(1,809)	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	1:38:D:PRO:N	10	5.08
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	18	5.07
(1,299)	1:33:B:GLN:N	1:33:B:GLN:CA	1:33:B:GLN:C	1:34:B:LYS:N	12	5.07
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	11	5.06
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	5	5.02
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	3	5.0
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	4	4.99
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	10	4.98
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	11	4.97
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	2	4.97
(1,750)	1:137:C:PHE:C	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	16	4.96
(1,375)	1:72:B:THR:N	1:72:B:THR:CA	1:72:B:THR:C	1:73:B:ALA:N	5	4.96
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	19	4.96
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	10	4.95
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	7	4.94
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	18	4.94
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	9	4.91
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	3	4.91
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	5	4.91
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	20	4.91
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	12	4.9
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	18	4.9
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	17	4.9
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	11	4.9
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	2	4.88
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	7	4.88
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	12	4.88
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	9	4.87
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	5	4.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	15	4.86
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	19	4.86
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	9	4.86
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	20	4.85
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	11	4.84
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	15	4.84
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	7	4.82
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	15	4.82
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	10	4.82
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	7	4.79
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	8	4.76
(1,767)	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	1:15:D:ARG:N	12	4.76
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	20	4.76
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	18	4.75
(1,749)	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	1:138:C:MET:N	9	4.75
(1,411)	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	1:91:B:GLY:N	1	4.75
(1,375)	1:72:B:THR:N	1:72:B:THR:CA	1:72:B:THR:C	1:73:B:ALA:N	14	4.75
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	5	4.74
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	10	4.72
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	14	4.72
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	18	4.71
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	10	4.69
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	11	4.69
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	11	4.69
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	9	4.68
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	5	4.67
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	8	4.66
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	7	4.66
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	14	4.66
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	17	4.66
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	9	4.65
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	13	4.64
(1,306)	1:36:B:TRP:C	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	17	4.64
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	16	4.64
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	7	4.64
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	8	4.63
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	9	4.62
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	1	4.62
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	4	4.61
(1,302)	1:34:B:LYS:C	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	9	4.57
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	11	4.57
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	7	4.56
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	14	4.56
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	3	4.56
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	6	4.55
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	8	4.54
(1,750)	1:137:C:PHE:C	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	15	4.54
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	18	4.49
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1	4.48
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	19	4.46
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	2	4.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	13	4.45
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	12	4.44
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	20	4.44
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	3	4.43
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	6	4.43
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	16	4.42
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	14	4.42
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	7	4.42
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	1	4.39
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	13	4.39
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	12	4.38
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	15	4.36
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	18	4.36
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	3	4.36
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	20	4.36
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	17	4.36
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	12	4.36
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	4	4.35
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	15	4.35
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	12	4.35
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	7	4.34
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	19	4.34
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	17	4.32
(1,302)	1:34:B:LYS:C	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	20	4.32
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	12	4.32
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	20	4.31
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	12	4.3
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	11	4.3
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	15	4.29
(1,830)	1:48:D:SER:C	1:49:D:SER:N	1:49:D:SER:CA	1:49:D:SER:C	18	4.28
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	14	4.28
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	17	4.27
(1,767)	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	1:15:D:ARG:N	19	4.27
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	20	4.27
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	5	4.27
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	14	4.27
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	13	4.27
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	18	4.27
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	17	4.26
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	5	4.25
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	12	4.25
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	7	4.25
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	17	4.23
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	13	4.23
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	6	4.22
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	12	4.22
(1,599)	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	1:59:C:VAL:N	3	4.21
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	16	4.2
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	9	4.2
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	10	4.2
(1,305)	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1:37:B:GLN:N	1	4.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	3	4.19
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	18	4.19
(1,86)	1:54:A:ASP:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	6	4.19
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	1	4.19
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	4	4.18
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	19	4.18
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	5	4.18
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	3	4.18
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	12	4.16
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	10	4.15
(1,823)	1:45:D:ASP:N	1:45:D:ASP:CA	1:45:D:ASP:C	1:46:D:THR:N	1	4.15
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	18	4.14
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	15	4.13
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	16	4.12
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	3	4.12
(1,977)	1:125:D:GLN:N	1:125:D:GLN:CA	1:125:D:GLN:C	1:126:D:LEU:N	20	4.1
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	10	4.09
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	14	4.09
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	3	4.07
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	9	4.07
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	17	4.07
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	3	4.07
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	3	4.07
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	16	4.06
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	3	4.05
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	8	4.04
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	14	4.04
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	14	4.03
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	12	4.02
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	18	4.01
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	9	4.0
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	7	4.0
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	10	3.97
(1,977)	1:125:D:GLN:N	1:125:D:GLN:CA	1:125:D:GLN:C	1:126:D:LEU:N	18	3.96
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	1	3.96
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	20	3.96
(1,370)	1:69:B:GLY:C	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	4	3.96
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	6	3.94
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	6	3.93
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	15	3.93
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	7	3.92
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	1	3.92
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	17	3.91
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	11	3.91
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	16	3.91
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	8	3.91
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	8	3.9
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	2	3.9
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	2	3.9
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1	3.9
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	9	3.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	6	3.87
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	18	3.86
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	1	3.86
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	4	3.86
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	11	3.86
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	9	3.86
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	3	3.84
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	17	3.84
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	16	3.84
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	20	3.84
(1,915)	1:91:D:GLY:N	1:91:D:GLY:CA	1:91:D:GLY:C	1:92:D:THR:N	12	3.83
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	3	3.82
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	5	3.82
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	4	3.81
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	3	3.81
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	14	3.8
(1,367)	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	1:69:B:GLY:N	17	3.8
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	20	3.8
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1	3.8
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	15	3.79
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	14	3.78
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	2	3.78
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	20	3.77
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	5	3.77
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	1	3.76
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	11	3.76
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	18	3.76
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	1	3.75
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	6	3.75
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	13	3.74
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	17	3.74
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	6	3.74
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	1	3.73
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	2	3.73
(1,767)	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	1:15:D:ARG:N	8	3.72
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	12	3.72
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	16	3.72
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	8	3.72
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	7	3.72
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	12	3.72
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	8	3.71
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	3	3.71
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1	3.71
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	20	3.71
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	13	3.7
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	6	3.7
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	12	3.7
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	5	3.68
(1,767)	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	1:15:D:ARG:N	9	3.68
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	15	3.67
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	16	3.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	20	3.67
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	18	3.67
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	3	3.67
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	15	3.66
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	4	3.66
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	13	3.66
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	17	3.65
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	14	3.65
(1,739)	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	1:133:C:PHE:N	19	3.65
(1,535)	1:23:C:PHE:N	1:23:C:PHE:CA	1:23:C:PHE:C	1:24:C:GLU:N	6	3.65
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	6	3.65
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	20	3.63
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	17	3.63
(1,299)	1:33:B:GLN:N	1:33:B:GLN:CA	1:33:B:GLN:C	1:34:B:LYS:N	7	3.63
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	10	3.63
(1,784)	1:22:D:SER:C	1:23:D:PHE:N	1:23:D:PHE:CA	1:23:D:PHE:C	19	3.61
(1,784)	1:22:D:SER:C	1:23:D:PHE:N	1:23:D:PHE:CA	1:23:D:PHE:C	20	3.61
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	3	3.59
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	5	3.59
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	10	3.59
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	13	3.58
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	16	3.58
(1,264)	1:13:B:ILE:C	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	17	3.57
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	12	3.56
(1,252)	1:141:A:LEU:C	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	3	3.56
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	20	3.55
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	17	3.55
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	19	3.55
(1,61)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:ASP:N	6	3.55
(1,412)	1:90:B:GLU:C	1:91:B:GLY:N	1:91:B:GLY:CA	1:91:B:GLY:C	1	3.54
(1,32)	1:24:A:GLU:C	1:25:A:ALA:N	1:25:A:ALA:CA	1:25:A:ALA:C	2	3.54
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	15	3.53
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	11	3.53
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	6	3.53
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	14	3.52
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	5	3.52
(1,55)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:VAL:N	18	3.52
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	15	3.51
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	6	3.51
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	6	3.51
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	3	3.51
(1,1006)	1:140:D:TYR:C	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	5	3.5
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	1	3.5
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	14	3.5
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	4	3.5
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	4	3.5
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	1	3.49
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	6	3.48
(1,165)	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	1:95:A:ALA:N	17	3.48
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	8	3.48
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	4	3.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	3	3.47
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	16	3.46
(1,799)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:GLN:N	19	3.46
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	8	3.46
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	2	3.45
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	17	3.45
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	18	3.45
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	15	3.44
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	8	3.44
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	11	3.44
(1,76)	1:49:A:SER:C	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	11	3.44
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	12	3.43
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	4	3.42
(1,808)	1:36:D:TRP:C	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	15	3.42
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	15	3.42
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1	3.42
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	4	3.42
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	9	3.41
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	11	3.41
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	6	3.41
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	9	3.41
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	18	3.41
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	1	3.41
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	14	3.4
(1,883)	1:75:D:LEU:N	1:75:D:LEU:CA	1:75:D:LEU:C	1:76:D:CYS:N	14	3.4
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	6	3.4
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	11	3.4
(1,558)	1:36:C:TRP:C	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	8	3.4
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	9	3.4
(1,152)	1:87:A:ALA:C	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	11	3.4
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	5	3.39
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	7	3.39
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	5	3.39
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	4	3.39
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	18	3.39
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	11	3.39
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	17	3.38
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	19	3.38
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	12	3.37
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	15	3.37
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	14	3.37
(1,673)	1:95:C:ALA:N	1:95:C:ALA:CA	1:95:C:ALA:C	1:96:C:HIS:N	10	3.36
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	19	3.36
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	8	3.35
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	7	3.35
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	15	3.35
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	19	3.35
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	19	3.34
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	6	3.34
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	1	3.33
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	18	3.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	5	3.33
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	1	3.33
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	15	3.33
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	16	3.33
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	2	3.32
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	4	3.32
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	10	3.32
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	19	3.31
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	5	3.31
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	17	3.3
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	10	3.3
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	17	3.28
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	8	3.28
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	8	3.28
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	17	3.28
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	5	3.28
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	1	3.27
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	6	3.27
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	12	3.26
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	6	3.26
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	10	3.26
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	11	3.26
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	15	3.25
(1,741)	1:133:C:PHE:N	1:133:C:PHE:CA	1:133:C:PHE:C	1:134:C:ASP:N	18	3.25
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	2	3.25
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	19	3.25
(1,766)	1:13:D:ILE:C	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	4	3.24
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	17	3.24
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	6	3.24
(1,665)	1:91:C:GLY:N	1:91:C:GLY:CA	1:91:C:GLY:C	1:92:C:THR:N	2	3.23
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	1	3.22
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	14	3.22
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	2	3.22
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	14	3.22
(1,28)	1:22:A:SER:C	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	20	3.22
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	6	3.21
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	6	3.21
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	18	3.21
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	18	3.2
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	8	3.2
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	9	3.19
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	11	3.19
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	3	3.19
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	9	3.19
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	17	3.19
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	17	3.19
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	5	3.18
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	9	3.17
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	19	3.17
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	14	3.17
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	3	3.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	11	3.16
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	19	3.16
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	9	3.15
(1,607)	1:62:C:VAL:N	1:62:C:VAL:CA	1:62:C:VAL:C	1:63:C:THR:N	18	3.15
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	7	3.15
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	17	3.15
(1,105)	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1:65:A:THR:N	15	3.15
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	3	3.14
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	11	3.14
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	3	3.14
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	8	3.14
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	19	3.14
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	13	3.14
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	18	3.14
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	4	3.13
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	6	3.13
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	12	3.13
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	13	3.13
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	7	3.12
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	2	3.12
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	8	3.12
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	7	3.12
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	15	3.12
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	13	3.12
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	1	3.12
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	17	3.12
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	12	3.11
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	9	3.11
(1,758)	1:9:D:MET:C	1:10:D:THR:N	1:10:D:THR:CA	1:10:D:THR:C	4	3.11
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	1	3.11
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	9	3.11
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	14	3.11
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	13	3.1
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	13	3.09
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	10	3.09
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	4	3.09
(1,14)	1:15:A:ARG:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	6	3.09
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	13	3.08
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	2	3.08
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	18	3.07
(1,376)	1:72:B:THR:C	1:73:B:ALA:N	1:73:B:ALA:CA	1:73:B:ALA:C	11	3.07
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	8	3.07
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	6	3.07
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	9	3.06
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	14	3.06
(1,660)	1:88:C:GLY:C	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	6	3.06
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	8	3.06
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	2	3.06
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	18	3.06
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	15	3.05
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	4	3.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	18	3.05
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	14	3.05
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	10	3.05
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	6	3.05
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	13	3.04
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	19	3.04
(1,542)	1:27:C:ASN:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	15	3.04
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	3	3.04
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	14	3.04
(1,401)	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	1:86:B:ILE:N	17	3.03
(1,146)	1:84:A:PHE:C	1:85:A:SER:N	1:85:A:SER:CA	1:85:A:SER:C	2	3.03
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	10	3.02
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	18	3.02
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	11	3.02
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	18	3.02
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	19	3.02
(1,76)	1:49:A:SER:C	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	9	3.02
(1,570)	1:43:C:ASP:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	19	3.01
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	6	3.01
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	20	3.01
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	8	3.0
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	1	3.0
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	4	3.0
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	17	3.0
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	16	3.0
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	12	3.0
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	8	2.99
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	3	2.99
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	3	2.99
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	12	2.98
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	11	2.98
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	11	2.98
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	4	2.98
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	6	2.98
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	1	2.97
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	15	2.97
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	16	2.97
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	2	2.97
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	20	2.97
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	16	2.97
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1	2.97
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	7	2.96
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	9	2.96
(1,733)	1:128:C:LEU:N	1:128:C:LEU:CA	1:128:C:LEU:C	1:129:C:ALA:N	5	2.96
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	20	2.96
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	12	2.95
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	3	2.95
(1,503)	1:140:B:TYR:N	1:140:B:TYR:CA	1:140:B:TYR:C	1:141:B:LEU:N	5	2.95
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	13	2.95
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	8	2.95
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	9	2.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,808)	1:36:D:TRP:C	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	20	2.94
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	4	2.94
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	5	2.94
(1,383)	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	1:77:B:GLU:N	11	2.94
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	12	2.94
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	7	2.94
(1,224)	1:126:A:LEU:C	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	19	2.94
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	20	2.93
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	8	2.93
(1,571)	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	1:45:C:ASP:N	9	2.93
(1,352)	1:60:B:LEU:C	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	14	2.93
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	7	2.92
(1,728)	1:125:C:GLN:C	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	6	2.92
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	20	2.92
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	6	2.92
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	12	2.92
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	20	2.92
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	2	2.91
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	15	2.91
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	4	2.91
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	1	2.91
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	4	2.91
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	16	2.9
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	10	2.9
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	17	2.9
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	14	2.9
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	14	2.9
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	16	2.89
(1,30)	1:23:A:PHE:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	20	2.89
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	15	2.88
(1,149)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:ALA:N	19	2.88
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	20	2.88
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	5	2.88
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	6	2.87
(1,217)	1:122:A:THR:N	1:122:A:THR:CA	1:122:A:THR:C	1:123:A:PHE:N	5	2.87
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	8	2.86
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	12	2.86
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	16	2.85
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	10	2.85
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	4	2.85
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	9	2.85
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	19	2.84
(1,767)	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	1:15:D:ARG:N	20	2.84
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	20	2.84
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	5	2.84
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	5	2.84
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	4	2.84
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	6	2.83
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	15	2.83
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	2	2.83
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	17	2.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,409)	1:89:B:ILE:N	1:89:B:ILE:CA	1:89:B:ILE:C	1:90:B:GLU:N	2	2.83
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	3	2.83
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	11	2.82
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	1	2.82
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	17	2.82
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	18	2.82
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	8	2.82
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	7	2.81
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	15	2.81
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	18	2.81
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	20	2.81
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	20	2.81
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	16	2.8
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	19	2.8
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	12	2.8
(1,727)	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1:126:C:LEU:N	16	2.8
(1,621)	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	1:70:C:GLU:N	17	2.8
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	1	2.8
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	14	2.8
(1,724)	1:122:C:THR:C	1:123:C:PHE:N	1:123:C:PHE:CA	1:123:C:PHE:C	18	2.79
(1,623)	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1:71:C:GLU:N	6	2.79
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	2	2.79
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	19	2.79
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	9	2.78
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	15	2.78
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	8	2.78
(1,731)	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	1:128:C:LEU:N	14	2.78
(1,542)	1:27:C:ASN:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	4	2.78
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	11	2.77
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	15	2.77
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	4	2.76
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	8	2.76
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	1	2.76
(1,787)	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	1:25:D:ALA:N	10	2.75
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	19	2.75
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	4	2.75
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	1	2.75
(1,800)	1:32:D:PHE:C	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	18	2.74
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	8	2.73
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	4	2.73
(1,788)	1:24:D:GLU:C	1:25:D:ALA:N	1:25:D:ALA:CA	1:25:D:ALA:C	10	2.73
(1,727)	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1:126:C:LEU:N	2	2.73
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	20	2.73
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	2	2.73
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	19	2.73
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	15	2.73
(1,35)	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1:28:A:ALA:N	17	2.73
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	10	2.72
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	16	2.72
(1,375)	1:72:B:THR:N	1:72:B:THR:CA	1:72:B:THR:C	1:73:B:ALA:N	10	2.71
(1,119)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:THR:N	10	2.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	18	2.7
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	4	2.7
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	19	2.7
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	17	2.7
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	9	2.7
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	9	2.7
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	7	2.7
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	3	2.7
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	5	2.69
(1,623)	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1:71:C:GLU:N	10	2.69
(1,367)	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	1:69:B:GLY:N	18	2.69
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	15	2.69
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	6	2.69
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	8	2.69
(1,126)	1:74:A:PHE:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1	2.69
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	11	2.69
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	11	2.69
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	18	2.68
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	11	2.68
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	6	2.68
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	5	2.68
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	15	2.68
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	9	2.68
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	20	2.67
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	11	2.67
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	11	2.67
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	14	2.67
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	16	2.67
(1,91)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:VAL:N	6	2.67
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	12	2.66
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	20	2.66
(1,289)	1:27:B:ASN:N	1:27:B:ASN:CA	1:27:B:ASN:C	1:28:B:ALA:N	1	2.66
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	2	2.66
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	8	2.66
(1,10)	1:13:A:ILE:C	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	19	2.66
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	5	2.65
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	15	2.65
(1,558)	1:36:C:TRP:C	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	15	2.65
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	15	2.65
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	20	2.65
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	6	2.65
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	7	2.65
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	18	2.65
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	11	2.64
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	16	2.64
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	2	2.64
(1,407)	1:88:B:GLY:N	1:88:B:GLY:CA	1:88:B:GLY:C	1:89:B:ILE:N	1	2.64
(1,375)	1:72:B:THR:N	1:72:B:THR:CA	1:72:B:THR:C	1:73:B:ALA:N	7	2.64
(1,561)	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	1:40:C:VAL:N	12	2.63
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	19	2.63
(1,535)	1:23:C:PHE:N	1:23:C:PHE:CA	1:23:C:PHE:C	1:24:C:GLU:N	16	2.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	3	2.63
(1,75)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLN:N	7	2.63
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	12	2.62
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	11	2.62
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	11	2.62
(1,302)	1:34:B:LYS:C	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	10	2.62
(1,1003)	1:139:D:ASN:N	1:139:D:ASN:CA	1:139:D:ASN:C	1:140:D:TYR:N	8	2.61
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	12	2.61
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	8	2.61
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	19	2.61
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	11	2.61
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	20	2.61
(1,302)	1:34:B:LYS:C	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	7	2.61
(1,156)	1:89:A:ILE:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	10	2.61
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	1	2.61
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	4	2.6
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	4	2.6
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	1	2.6
(1,603)	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	1:61:C:ARG:N	8	2.6
(1,282)	1:22:B:SER:C	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	13	2.6
(1,219)	1:123:A:PHE:N	1:123:A:PHE:CA	1:123:A:PHE:C	1:124:A:PRO:N	5	2.6
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	7	2.6
(1,910)	1:88:D:GLY:C	1:89:D:ILE:N	1:89:D:ILE:CA	1:89:D:ILE:C	1	2.59
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	10	2.59
(1,538)	1:24:C:GLU:C	1:25:C:ALA:N	1:25:C:ALA:CA	1:25:C:ALA:C	14	2.59
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	6	2.59
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	5	2.58
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	11	2.58
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	2	2.58
(1,287)	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	1:26:B:PRO:N	9	2.58
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	6	2.58
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	4	2.58
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	2	2.58
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	14	2.58
(1,830)	1:48:D:SER:C	1:49:D:SER:N	1:49:D:SER:CA	1:49:D:SER:C	16	2.57
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	14	2.57
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	11	2.57
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	8	2.57
(1,310)	1:39:B:GLU:C	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	6	2.57
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	17	2.57
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	9	2.57
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	11	2.56
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	9	2.56
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	19	2.56
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	14	2.56
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	9	2.56
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	19	2.56
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	14	2.56
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	20	2.55
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	18	2.55
(1,347)	1:58:B:VAL:N	1:58:B:VAL:CA	1:58:B:VAL:C	1:59:B:VAL:N	2	2.55

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	6	2.55
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	16	2.55
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	17	2.54
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	15	2.53
(1,914)	1:90:D:GLU:C	1:91:D:GLY:N	1:91:D:GLY:CA	1:91:D:GLY:C	12	2.53
(1,287)	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	1:26:B:PRO:N	3	2.53
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	5	2.53
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	13	2.53
(1,915)	1:91:D:GLY:N	1:91:D:GLY:CA	1:91:D:GLY:C	1:92:D:THR:N	10	2.52
(1,626)	1:71:C:GLU:C	1:72:C:THR:N	1:72:C:THR:CA	1:72:C:THR:C	2	2.52
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	20	2.52
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	11	2.52
(1,105)	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1:65:A:THR:N	13	2.52
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	10	2.51
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	12	2.51
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	1	2.51
(1,393)	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1:82:B:GLY:N	5	2.51
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	10	2.51
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	15	2.51
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	3	2.5
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	7	2.5
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	7	2.5
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	18	2.5
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	1	2.5
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	16	2.5
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	17	2.49
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	10	2.49
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	7	2.49
(1,308)	1:38:B:PRO:C	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	19	2.49
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	6	2.49
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	19	2.49
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	3	2.49
(1,783)	1:22:D:SER:N	1:22:D:SER:CA	1:22:D:SER:C	1:23:D:PHE:N	19	2.48
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	14	2.48
(1,372)	1:70:B:GLU:C	1:71:B:GLU:N	1:71:B:GLU:CA	1:71:B:GLU:C	4	2.48
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	1	2.47
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	11	2.47
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	17	2.47
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	12	2.47
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	11	2.47
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	6	2.46
(1,709)	1:115:C:THR:N	1:115:C:THR:CA	1:115:C:THR:C	1:116:C:SER:N	15	2.46
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	20	2.46
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	7	2.45
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	13	2.45
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	9	2.45
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	17	2.45
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	11	2.45
(1,738)	1:131:C:VAL:C	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	19	2.44
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	18	2.44
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	7	2.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	2	2.44
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	16	2.44
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	7	2.44
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	10	2.44
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	9	2.43
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	4	2.43
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	2	2.43
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	4	2.43
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	13	2.42
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	7	2.42
(1,575)	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	1:47:C:ALA:N	13	2.42
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	18	2.42
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	3	2.42
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	8	2.42
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	15	2.42
(1,32)	1:24:A:GLU:C	1:25:A:ALA:N	1:25:A:ALA:CA	1:25:A:ALA:C	13	2.42
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	12	2.41
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	11	2.41
(1,538)	1:24:C:GLU:C	1:25:C:ALA:N	1:25:C:ALA:CA	1:25:C:ALA:C	20	2.41
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	13	2.41
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	3	2.41
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	5	2.41
(1,345)	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	1:58:B:VAL:N	18	2.41
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	13	2.41
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	7	2.41
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	18	2.4
(1,832)	1:49:D:SER:C	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	18	2.4
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	19	2.4
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	10	2.4
(1,400)	1:84:B:PHE:C	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	18	2.4
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	3	2.4
(1,315)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:ASP:N	7	2.4
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	14	2.4
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	14	2.39
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	3	2.39
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	11	2.39
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	4	2.39
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	11	2.39
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	4	2.39
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	13	2.39
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	16	2.39
(1,797)	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	1:32:D:PHE:N	14	2.38
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	18	2.38
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	9	2.38
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	20	2.38
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	16	2.38
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	4	2.38
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	17	2.37
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	10	2.37
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	14	2.37
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	10	2.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	14	2.37
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	8	2.37
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	20	2.36
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	13	2.36
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	1	2.36
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	10	2.36
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	12	2.36
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	11	2.36
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	4	2.35
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	16	2.35
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	18	2.35
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	8	2.35
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	7	2.35
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	2	2.35
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	12	2.35
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	4	2.35
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	9	2.34
(1,660)	1:88:C:GLY:C	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	12	2.34
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	13	2.34
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	16	2.34
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	20	2.33
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	14	2.33
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	13	2.33
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	6	2.33
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1	2.33
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	17	2.33
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	9	2.33
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	7	2.33
(1,804)	1:34:D:LYS:C	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	8	2.32
(1,797)	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	1:32:D:PHE:N	10	2.32
(1,784)	1:22:D:SER:C	1:23:D:PHE:N	1:23:D:PHE:CA	1:23:D:PHE:C	8	2.32
(1,734)	1:128:C:LEU:C	1:129:C:ALA:N	1:129:C:ALA:CA	1:129:C:ALA:C	15	2.32
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	18	2.32
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	6	2.32
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	10	2.32
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	10	2.31
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	10	2.31
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	18	2.31
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	5	2.31
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	8	2.31
(1,77)	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	1:51:A:LEU:N	10	2.31
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	3	2.31
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	13	2.3
(1,575)	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	1:47:C:ALA:N	2	2.3
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	15	2.3
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	19	2.3
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	13	2.3
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	18	2.3
(1,130)	1:76:A:CYS:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	10	2.3
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	5	2.3
(1,929)	1:98:D:LEU:N	1:98:D:LEU:CA	1:98:D:LEU:C	1:99:D:GLY:N	9	2.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	10	2.29
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	17	2.29
(1,352)	1:60:B:LEU:C	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	8	2.29
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	16	2.29
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	17	2.29
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	16	2.28
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	13	2.28
(1,290)	1:27:B:ASN:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	6	2.28
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	10	2.28
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	13	2.28
(1,61)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:ASP:N	16	2.28
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	20	2.27
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	10	2.27
(1,76)	1:49:A:SER:C	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	12	2.27
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	16	2.27
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	2	2.27
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	8	2.26
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	8	2.26
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	9	2.26
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	17	2.26
(1,290)	1:27:B:ASN:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	5	2.26
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	4	2.26
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	6	2.26
(1,30)	1:23:A:PHE:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	15	2.26
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	19	2.25
(1,559)	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	1:38:C:PRO:N	1	2.25
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	14	2.25
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	18	2.25
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	7	2.24
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	8	2.24
(1,767)	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	1:15:D:ARG:N	5	2.24
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	3	2.24
(1,281)	1:22:B:SER:N	1:22:B:SER:CA	1:22:B:SER:C	1:23:B:PHE:N	13	2.24
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	19	2.24
(1,225)	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	1:128:A:LEU:N	2	2.24
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	11	2.24
(1,983)	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	1:129:D:ALA:N	2	2.23
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	11	2.23
(1,222)	1:125:A:GLN:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	13	2.23
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	9	2.23
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	12	2.22
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	19	2.22
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	4	2.22
(1,648)	1:82:C:GLY:C	1:83:C:ILE:N	1:83:C:ILE:CA	1:83:C:ILE:C	5	2.22
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	16	2.22
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	3	2.22
(1,406)	1:87:B:ALA:C	1:88:B:GLY:N	1:88:B:GLY:CA	1:88:B:GLY:C	10	2.22
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	20	2.22
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	3	2.22
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	2	2.21
(1,673)	1:95:C:ALA:N	1:95:C:ALA:CA	1:95:C:ALA:C	1:96:C:HIS:N	9	2.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,631)	1:74:C:PHE:N	1:74:C:PHE:CA	1:74:C:PHE:C	1:75:C:LEU:N	12	2.21
(1,557)	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	1:37:C:GLN:N	8	2.21
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	9	2.21
(1,519)	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	1:16:C:ILE:N	15	2.21
(1,476)	1:125:B:GLN:C	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	15	2.21
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	8	2.21
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	1	2.21
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	18	2.21
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	14	2.2
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	3	2.2
(1,883)	1:75:D:LEU:N	1:75:D:LEU:CA	1:75:D:LEU:C	1:76:D:CYS:N	2	2.2
(1,806)	1:35:D:ASP:C	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	20	2.2
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	8	2.2
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	4	2.2
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	1	2.2
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	16	2.2
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	6	2.2
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	6	2.19
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	11	2.19
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	19	2.19
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	3	2.19
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	4	2.19
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	20	2.19
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	17	2.18
(1,542)	1:27:C:ASN:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	8	2.18
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	1	2.18
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	14	2.18
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	17	2.18
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1	2.18
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	20	2.18
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	20	2.18
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	1	2.17
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	15	2.17
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	2	2.17
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	7	2.17
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	11	2.17
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	16	2.17
(1,375)	1:72:B:THR:N	1:72:B:THR:CA	1:72:B:THR:C	1:73:B:ALA:N	19	2.17
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	6	2.16
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	5	2.16
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	13	2.16
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	5	2.16
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	17	2.15
(1,621)	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	1:70:C:GLU:N	20	2.15
(1,574)	1:45:C:ASP:C	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	5	2.15
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	18	2.15
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	3	2.15
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	18	2.15
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	5	2.14
(1,872)	1:69:D:GLY:C	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	20	2.14
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	12	2.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,820)	1:43:D:ASP:C	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	6	2.14
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	12	2.14
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	17	2.14
(1,55)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:VAL:N	9	2.14
(1,9)	1:13:A:ILE:N	1:13:A:ILE:CA	1:13:A:ILE:C	1:14:A:GLN:N	19	2.14
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	18	2.13
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	6	2.13
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	10	2.13
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	11	2.13
(1,316)	1:42:B:LEU:C	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	10	2.13
(1,307)	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	1:38:B:PRO:N	16	2.13
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	11	2.13
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	19	2.13
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	6	2.13
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	4	2.12
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	7	2.12
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	9	2.12
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	12	2.12
(1,411)	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	1:91:B:GLY:N	4	2.12
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	2	2.12
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	6	2.12
(1,109)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:SER:N	15	2.12
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1	2.12
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	3	2.12
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	3	2.11
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	10	2.11
(1,635)	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1:77:C:GLU:N	14	2.11
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	18	2.11
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	11	2.11
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	20	2.11
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	7	2.11
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	17	2.11
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	19	2.11
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	16	2.1
(1,600)	1:58:C:VAL:C	1:59:C:VAL:N	1:59:C:VAL:CA	1:59:C:VAL:C	8	2.1
(1,581)	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	1:50:C:GLN:N	6	2.1
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	20	2.1
(1,350)	1:59:B:VAL:C	1:60:B:LEU:N	1:60:B:LEU:CA	1:60:B:LEU:C	10	2.1
(1,248)	1:139:A:ASN:C	1:140:A:TYR:N	1:140:A:TYR:CA	1:140:A:TYR:C	7	2.1
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	14	2.1
(1,226)	1:127:A:ASN:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	18	2.1
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	9	2.1
(1,830)	1:48:D:SER:C	1:49:D:SER:N	1:49:D:SER:CA	1:49:D:SER:C	20	2.09
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	16	2.09
(1,574)	1:45:C:ASP:C	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	2	2.09
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	11	2.09
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	3	2.09
(1,86)	1:54:A:ASP:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	3	2.09
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	7	2.09
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	16	2.09
(1,815)	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	1:42:D:LEU:N	13	2.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1	2.08
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	6	2.08
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	6	2.08
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	20	2.08
(1,105)	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1:65:A:THR:N	5	2.08
(1,635)	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1:77:C:GLU:N	20	2.07
(1,542)	1:27:C:ASN:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	1	2.07
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	2	2.07
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	7	2.07
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	9	2.07
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	12	2.06
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	5	2.06
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	18	2.06
(1,754)	1:139:C:ASN:C	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	11	2.05
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	9	2.05
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	13	2.05
(1,386)	1:77:B:GLU:C	1:78:B:VAL:N	1:78:B:VAL:CA	1:78:B:VAL:C	11	2.05
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	19	2.05
(1,38)	1:29:A:PRO:C	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	17	2.05
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	5	2.04
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	8	2.04
(1,400)	1:84:B:PHE:C	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	10	2.04
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	4	2.04
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	4	2.04
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1	2.04
(1,912)	1:89:D:ILE:C	1:90:D:GLU:N	1:90:D:GLU:CA	1:90:D:GLU:C	11	2.03
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	12	2.03
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	3	2.03
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	9	2.03
(1,578)	1:47:C:ALA:C	1:48:C:SER:N	1:48:C:SER:CA	1:48:C:SER:C	20	2.03
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	11	2.03
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	6	2.03
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	12	2.02
(1,552)	1:33:C:GLN:C	1:34:C:LYS:N	1:34:C:LYS:CA	1:34:C:LYS:C	15	2.02
(1,542)	1:27:C:ASN:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	10	2.02
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	7	2.02
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	4	2.02
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	20	2.02
(1,290)	1:27:B:ASN:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	18	2.02
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	1	2.02
(1,106)	1:64:A:VAL:C	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	9	2.02
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	4	2.01
(1,911)	1:89:D:ILE:N	1:89:D:ILE:CA	1:89:D:ILE:C	1:90:D:GLU:N	17	2.01
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	17	2.01
(1,832)	1:49:D:SER:C	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	20	2.01
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	14	2.01
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	18	2.01
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	9	2.01
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	19	2.0
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	12	2.0
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	9	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	8	2.0
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	3	2.0
(1,1006)	1:140:D:TYR:C	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	8	1.99
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	9	1.99
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	13	1.99
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	19	1.99
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	19	1.99
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	19	1.99
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	15	1.99
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	4	1.99
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	14	1.99
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	1	1.99
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	10	1.99
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	13	1.99
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	11	1.99
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	7	1.98
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	5	1.98
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	5	1.98
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	9	1.98
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	1	1.98
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	20	1.98
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	4	1.98
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	13	1.97
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	13	1.97
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	10	1.97
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	5	1.97
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	6	1.97
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	7	1.97
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	3	1.96
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	8	1.96
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	17	1.96
(1,556)	1:35:C:ASP:C	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	15	1.96
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	9	1.96
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	5	1.96
(1,272)	1:17:B:TYR:C	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	17	1.96
(1,169)	1:96:A:HIS:N	1:96:A:HIS:CA	1:96:A:HIS:C	1:97:A:CYS:N	17	1.96
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	18	1.96
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	12	1.96
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	13	1.96
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	17	1.95
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	5	1.95
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	4	1.95
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	9	1.95
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	12	1.95
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	11	1.95
(1,152)	1:87:A:ALA:C	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	19	1.95
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	13	1.95
(1,94)	1:58:A:VAL:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	13	1.95
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	14	1.95
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	18	1.94
(1,976)	1:124:D:PRO:C	1:125:D:GLN:N	1:125:D:GLN:CA	1:125:D:GLN:C	14	1.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	3	1.94
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	9	1.94
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	16	1.94
(1,223)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:ASN:N	12	1.94
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	8	1.94
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	13	1.94
(1,934)	1:100:D:ALA:C	1:101:D:TYR:N	1:101:D:TYR:CA	1:101:D:TYR:C	15	1.93
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	10	1.93
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	3	1.93
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	15	1.93
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	4	1.93
(1,731)	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	1:128:C:LEU:N	4	1.93
(1,607)	1:62:C:VAL:N	1:62:C:VAL:CA	1:62:C:VAL:C	1:63:C:THR:N	3	1.93
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	1	1.93
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1	1.93
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	15	1.93
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	9	1.93
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	13	1.92
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	10	1.92
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	4	1.92
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	5	1.92
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	5	1.92
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	13	1.92
(1,409)	1:89:B:ILE:N	1:89:B:ILE:CA	1:89:B:ILE:C	1:90:B:GLU:N	3	1.92
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	14	1.92
(1,934)	1:100:D:ALA:C	1:101:D:TYR:N	1:101:D:TYR:CA	1:101:D:TYR:C	3	1.91
(1,754)	1:139:C:ASN:C	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1	1.91
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	2	1.91
(1,723)	1:122:C:THR:N	1:122:C:THR:CA	1:122:C:THR:C	1:123:C:PHE:N	1	1.91
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	4	1.91
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	1	1.91
(1,353)	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	1:62:B:VAL:N	5	1.91
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	18	1.91
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	19	1.91
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	17	1.91
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	17	1.9
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	4	1.9
(1,602)	1:59:C:VAL:C	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	3	1.9
(1,536)	1:23:C:PHE:C	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	14	1.9
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	9	1.9
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	9	1.9
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	11	1.9
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	8	1.9
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	13	1.9
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	10	1.89
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	7	1.89
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	15	1.89
(1,653)	1:85:C:SER:N	1:85:C:SER:CA	1:85:C:SER:C	1:86:C:ILE:N	18	1.89
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	16	1.89
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	17	1.89
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	15	1.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,375)	1:72:B:THR:N	1:72:B:THR:CA	1:72:B:THR:C	1:73:B:ALA:N	12	1.89
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	19	1.89
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	1	1.89
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	2	1.89
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	7	1.89
(1,663)	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	1:91:C:GLY:N	14	1.88
(1,647)	1:82:C:GLY:N	1:82:C:GLY:CA	1:82:C:GLY:C	1:83:C:ILE:N	17	1.88
(1,581)	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	1:50:C:GLN:N	5	1.88
(1,69)	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1:47:A:ALA:N	20	1.88
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	2	1.88
(1,39)	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	1:31:A:VAL:N	15	1.88
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	18	1.88
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	11	1.87
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	17	1.87
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	3	1.87
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	4	1.87
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	4	1.87
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	2	1.87
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	14	1.87
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	5	1.87
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	11	1.86
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	9	1.86
(1,684)	1:100:C:ALA:C	1:101:C:TYR:N	1:101:C:TYR:CA	1:101:C:TYR:C	8	1.86
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	13	1.86
(1,581)	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	1:50:C:GLN:N	13	1.86
(1,562)	1:39:C:GLU:C	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	5	1.86
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	5	1.86
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	3	1.86
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	6	1.86
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	12	1.86
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	3	1.86
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1	1.86
(1,758)	1:9:D:MET:C	1:10:D:THR:N	1:10:D:THR:CA	1:10:D:THR:C	10	1.85
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	3	1.85
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	14	1.85
(1,999)	1:137:D:PHE:N	1:137:D:PHE:CA	1:137:D:PHE:C	1:138:D:MET:N	7	1.84
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	2	1.84
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	3	1.84
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	1	1.84
(1,288)	1:26:B:PRO:C	1:27:B:ASN:N	1:27:B:ASN:CA	1:27:B:ASN:C	16	1.84
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	20	1.84
(1,75)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLN:N	6	1.84
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	16	1.84
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	1	1.83
(1,738)	1:131:C:VAL:C	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	7	1.83
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	7	1.83
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	4	1.83
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1	1.83
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	9	1.83
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	4	1.83
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	8	1.83

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	4	1.82
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	11	1.82
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	10	1.82
(1,597)	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	1:58:C:VAL:N	6	1.82
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	16	1.82
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	8	1.82
(1,723)	1:122:C:THR:N	1:122:C:THR:CA	1:122:C:THR:C	1:123:C:PHE:N	9	1.81
(1,575)	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	1:47:C:ALA:N	5	1.81
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	10	1.81
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	19	1.81
(1,178)	1:100:A:ALA:C	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	6	1.81
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	12	1.81
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	5	1.81
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	10	1.81
(1,75)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLN:N	3	1.81
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	6	1.8
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	14	1.8
(1,352)	1:60:B:LEU:C	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	19	1.8
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	9	1.8
(1,53)	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1:38:A:PRO:N	5	1.8
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	20	1.79
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	6	1.79
(1,800)	1:32:D:PHE:C	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	14	1.79
(1,786)	1:23:D:PHE:C	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	19	1.79
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	5	1.79
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	12	1.79
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	20	1.79
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	9	1.79
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	4	1.79
(1,264)	1:13:B:ILE:C	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	15	1.79
(1,151)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLY:N	10	1.79
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	19	1.78
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	20	1.78
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	17	1.78
(1,299)	1:33:B:GLN:N	1:33:B:GLN:CA	1:33:B:GLN:C	1:34:B:LYS:N	18	1.78
(1,293)	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1:31:B:VAL:N	4	1.78
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	19	1.78
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	8	1.78
(1,55)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:VAL:N	8	1.78
(1,912)	1:89:D:ILE:C	1:90:D:GLU:N	1:90:D:GLU:CA	1:90:D:GLU:C	12	1.77
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	7	1.77
(1,684)	1:100:C:ALA:C	1:101:C:TYR:N	1:101:C:TYR:CA	1:101:C:TYR:C	12	1.77
(1,659)	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	1:89:C:ILE:N	16	1.77
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	8	1.77
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	9	1.77
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	11	1.77
(1,574)	1:45:C:ASP:C	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	11	1.77
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	6	1.77
(1,400)	1:84:B:PHE:C	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	12	1.77
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	10	1.77
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	14	1.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	20	1.77
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	13	1.77
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	12	1.77
(1,691)	1:105:C:ILE:N	1:105:C:ILE:CA	1:105:C:ILE:C	1:106:C:LEU:N	18	1.76
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	13	1.76
(1,612)	1:64:C:VAL:C	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	6	1.76
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	17	1.76
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	7	1.76
(1,106)	1:64:A:VAL:C	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	7	1.76
(1,28)	1:22:A:SER:C	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	15	1.76
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	11	1.75
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	18	1.75
(1,138)	1:80:A:GLN:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	3	1.75
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	7	1.75
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	19	1.74
(1,905)	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	1:87:D:ALA:N	5	1.74
(1,678)	1:97:C:CYS:C	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	11	1.74
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	20	1.74
(1,516)	1:13:C:ILE:C	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	18	1.74
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	19	1.74
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	9	1.74
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	16	1.74
(1,575)	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	1:47:C:ALA:N	12	1.73
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	2	1.73
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	15	1.73
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	12	1.73
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	20	1.73
(1,152)	1:87:A:ALA:C	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	6	1.73
(1,146)	1:84:A:PHE:C	1:85:A:SER:N	1:85:A:SER:CA	1:85:A:SER:C	8	1.73
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	13	1.73
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	8	1.73
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	15	1.73
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	19	1.73
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	4	1.72
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	13	1.72
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	5	1.72
(1,808)	1:36:D:TRP:C	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	10	1.72
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	19	1.72
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	12	1.72
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	13	1.72
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	14	1.72
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	15	1.72
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	8	1.72
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	11	1.71
(1,971)	1:121:D:GLY:N	1:121:D:GLY:CA	1:121:D:GLY:C	1:122:D:THR:N	13	1.71
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	17	1.71
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	12	1.71
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	8	1.71
(1,633)	1:75:C:LEU:N	1:75:C:LEU:CA	1:75:C:LEU:C	1:76:C:CYS:N	9	1.71
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	19	1.71
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	9	1.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,315)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:ASP:N	12	1.71
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	2	1.7
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	15	1.7
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	13	1.7
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	14	1.7
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	17	1.7
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	14	1.7
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	11	1.7
(1,237)	1:134:A:ASP:N	1:134:A:ASP:CA	1:134:A:ASP:C	1:135:A:ALA:N	1	1.7
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	17	1.7
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	12	1.7
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	1	1.69
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	3	1.69
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	20	1.69
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	7	1.69
(1,164)	1:93:A:GLN:C	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	8	1.69
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	10	1.68
(1,535)	1:23:C:PHE:N	1:23:C:PHE:CA	1:23:C:PHE:C	1:24:C:GLU:N	9	1.68
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	2	1.68
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	13	1.68
(1,138)	1:80:A:GLN:C	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	13	1.68
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	16	1.67
(1,865)	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	1:67:D:SER:N	15	1.67
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	7	1.67
(1,633)	1:75:C:LEU:N	1:75:C:LEU:CA	1:75:C:LEU:C	1:76:C:CYS:N	13	1.67
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	7	1.67
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	8	1.67
(1,504)	1:140:B:TYR:C	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	17	1.67
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	14	1.67
(1,267)	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	1:16:B:ILE:N	11	1.67
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	17	1.67
(1,149)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:ALA:N	7	1.67
(1,29)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	5	1.67
(1,989)	1:132:D:ASN:N	1:132:D:ASN:CA	1:132:D:ASN:C	1:133:D:PHE:N	12	1.66
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	19	1.66
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	18	1.66
(1,503)	1:140:B:TYR:N	1:140:B:TYR:CA	1:140:B:TYR:C	1:141:B:LEU:N	6	1.66
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	3	1.66
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	2	1.66
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	16	1.66
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	6	1.65
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	2	1.65
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	20	1.65
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	18	1.65
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	12	1.65
(1,852)	1:59:D:VAL:C	1:60:D:LEU:N	1:60:D:LEU:CA	1:60:D:LEU:C	20	1.64
(1,832)	1:49:D:SER:C	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	12	1.64
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	10	1.64
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	19	1.64
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	9	1.64
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	4	1.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	14	1.64
(1,214)	1:120:A:ARG:C	1:121:A:GLY:N	1:121:A:GLY:CA	1:121:A:GLY:C	15	1.64
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	5	1.64
(1,76)	1:49:A:SER:C	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	17	1.64
(1,934)	1:100:D:ALA:C	1:101:D:TYR:N	1:101:D:TYR:CA	1:101:D:TYR:C	10	1.63
(1,835)	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	1:52:D:ALA:N	3	1.63
(1,602)	1:59:C:VAL:C	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	15	1.63
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	9	1.63
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	1	1.63
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	9	1.63
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	18	1.63
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	5	1.63
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	11	1.62
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	19	1.62
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	19	1.62
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	5	1.62
(1,515)	1:13:C:ILE:N	1:13:C:ILE:CA	1:13:C:ILE:C	1:14:C:GLN:N	7	1.62
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	2	1.62
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	12	1.62
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	15	1.62
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	10	1.62
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	3	1.62
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	20	1.62
(1,848)	1:57:D:GLU:C	1:58:D:VAL:N	1:58:D:VAL:CA	1:58:D:VAL:C	5	1.61
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	20	1.61
(1,613)	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	1:66:C:ALA:N	18	1.61
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	6	1.61
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	2	1.61
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	18	1.61
(1,476)	1:125:B:GLN:C	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	7	1.61
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	17	1.61
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	11	1.61
(1,288)	1:26:B:PRO:C	1:27:B:ASN:N	1:27:B:ASN:CA	1:27:B:ASN:C	19	1.61
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	20	1.61
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	13	1.61
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	16	1.6
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	13	1.6
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	16	1.6
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	11	1.6
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	17	1.6
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	20	1.6
(1,137)	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	1:81:A:GLY:N	16	1.6
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	20	1.6
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	20	1.59
(1,797)	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	1:32:D:PHE:N	4	1.59
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1	1.59
(1,614)	1:65:C:THR:C	1:66:C:ALA:N	1:66:C:ALA:CA	1:66:C:ALA:C	14	1.59
(1,557)	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	1:37:C:GLN:N	13	1.59
(1,556)	1:35:C:ASP:C	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	18	1.59
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	3	1.59
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	12	1.59

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	4	1.59
(1,156)	1:89:A:ILE:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	6	1.59
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	20	1.59
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	2	1.59
(1,809)	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	1:38:D:PRO:N	14	1.58
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	2	1.58
(1,626)	1:71:C:GLU:C	1:72:C:THR:N	1:72:C:THR:CA	1:72:C:THR:C	3	1.58
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	6	1.58
(1,599)	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	1:59:C:VAL:N	6	1.58
(1,599)	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	1:59:C:VAL:N	7	1.58
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	19	1.58
(1,472)	1:122:B:THR:C	1:123:B:PHE:N	1:123:B:PHE:CA	1:123:B:PHE:C	13	1.58
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	2	1.58
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	5	1.58
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	1	1.58
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	2	1.58
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	19	1.58
(1,999)	1:137:D:PHE:N	1:137:D:PHE:CA	1:137:D:PHE:C	1:138:D:MET:N	3	1.57
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	16	1.57
(1,754)	1:139:C:ASN:C	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	10	1.57
(1,734)	1:128:C:LEU:C	1:129:C:ALA:N	1:129:C:ALA:CA	1:129:C:ALA:C	12	1.57
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	9	1.57
(1,128)	1:75:A:LEU:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	17	1.57
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	6	1.56
(1,822)	1:44:D:LEU:C	1:45:D:ASP:N	1:45:D:ASP:CA	1:45:D:ASP:C	12	1.56
(1,784)	1:22:D:SER:C	1:23:D:PHE:N	1:23:D:PHE:CA	1:23:D:PHE:C	12	1.56
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	7	1.56
(1,611)	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	1:65:C:THR:N	10	1.56
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	15	1.56
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	19	1.56
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	7	1.55
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	9	1.55
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	10	1.55
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	15	1.55
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	11	1.55
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	20	1.55
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	5	1.55
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	9	1.55
(1,263)	1:13:B:ILE:N	1:13:B:ILE:CA	1:13:B:ILE:C	1:14:B:GLN:N	12	1.55
(1,214)	1:120:A:ARG:C	1:121:A:GLY:N	1:121:A:GLY:CA	1:121:A:GLY:C	19	1.55
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	9	1.55
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	2	1.55
(1,105)	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1:65:A:THR:N	10	1.55
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	19	1.55
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	15	1.54
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	12	1.54
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	2	1.54
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	6	1.54
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	6	1.54
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	5	1.54
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	2	1.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	6	1.53
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	12	1.53
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	17	1.53
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	4	1.53
(1,671)	1:94:C:MET:N	1:94:C:MET:CA	1:94:C:MET:C	1:95:C:ALA:N	19	1.53
(1,229)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:PRO:N	10	1.53
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	11	1.53
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	20	1.52
(1,764)	1:12:D:GLN:C	1:13:D:ILE:N	1:13:D:ILE:CA	1:13:D:ILE:C	20	1.52
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	3	1.52
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	1	1.52
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	2	1.52
(1,352)	1:60:B:LEU:C	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	9	1.52
(1,348)	1:58:B:VAL:C	1:59:B:VAL:N	1:59:B:VAL:CA	1:59:B:VAL:C	8	1.52
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	2	1.52
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	3	1.52
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	6	1.52
(1,94)	1:58:A:VAL:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	5	1.52
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	8	1.51
(1,731)	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	1:128:C:LEU:N	12	1.51
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	13	1.51
(1,542)	1:27:C:ASN:C	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	11	1.51
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	17	1.51
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	4	1.51
(1,414)	1:91:B:GLY:C	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	8	1.51
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	13	1.51
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	8	1.51
(1,119)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:THR:N	3	1.51
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1	1.51
(1,903)	1:85:D:SER:N	1:85:D:SER:CA	1:85:D:SER:C	1:86:D:ILE:N	1	1.5
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	8	1.5
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	4	1.5
(1,631)	1:74:C:PHE:N	1:74:C:PHE:CA	1:74:C:PHE:C	1:75:C:LEU:N	11	1.5
(1,519)	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	1:16:C:ILE:N	12	1.5
(1,313)	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	1:42:B:LEU:N	2	1.5
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	20	1.5
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	9	1.49
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	12	1.49
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	2	1.49
(1,679)	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	1:99:C:GLY:N	12	1.49
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	20	1.49
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	2	1.49
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	4	1.49
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	6	1.49
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	16	1.49
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	6	1.49
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	5	1.49
(1,69)	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1:47:A:ALA:N	18	1.49
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	17	1.49
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	11	1.48
(1,903)	1:85:D:SER:N	1:85:D:SER:CA	1:85:D:SER:C	1:86:D:ILE:N	4	1.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,684)	1:100:C:ALA:C	1:101:C:TYR:N	1:101:C:TYR:CA	1:101:C:TYR:C	6	1.48
(1,647)	1:82:C:GLY:N	1:82:C:GLY:CA	1:82:C:GLY:C	1:83:C:ILE:N	18	1.48
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	8	1.48
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	3	1.48
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	2	1.48
(1,347)	1:58:B:VAL:N	1:58:B:VAL:CA	1:58:B:VAL:C	1:59:B:VAL:N	9	1.48
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	4	1.48
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	10	1.48
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	5	1.47
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	14	1.47
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	3	1.47
(1,883)	1:75:D:LEU:N	1:75:D:LEU:CA	1:75:D:LEU:C	1:76:D:CYS:N	13	1.47
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	10	1.47
(1,830)	1:48:D:SER:C	1:49:D:SER:N	1:49:D:SER:CA	1:49:D:SER:C	12	1.47
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	8	1.47
(1,550)	1:32:C:PHE:C	1:33:C:GLN:N	1:33:C:GLN:CA	1:33:C:GLN:C	17	1.47
(1,472)	1:122:B:THR:C	1:123:B:PHE:N	1:123:B:PHE:CA	1:123:B:PHE:C	9	1.47
(1,214)	1:120:A:ARG:C	1:121:A:GLY:N	1:121:A:GLY:CA	1:121:A:GLY:C	11	1.47
(1,53)	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1:38:A:PRO:N	11	1.47
(1,787)	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	1:25:D:ALA:N	12	1.46
(1,543)	1:28:C:ALA:N	1:28:C:ALA:CA	1:28:C:ALA:C	1:29:C:PRO:N	3	1.46
(1,403)	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1:87:B:ALA:N	16	1.46
(1,274)	1:18:B:THR:C	1:19:B:LYS:N	1:19:B:LYS:CA	1:19:B:LYS:C	13	1.46
(1,178)	1:100:A:ALA:C	1:101:A:TYR:N	1:101:A:TYR:CA	1:101:A:TYR:C	20	1.46
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	17	1.45
(1,875)	1:71:D:GLU:N	1:71:D:GLU:CA	1:71:D:GLU:C	1:72:D:THR:N	1	1.45
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	7	1.45
(1,808)	1:36:D:TRP:C	1:37:D:GLN:N	1:37:D:GLN:CA	1:37:D:GLN:C	19	1.45
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	7	1.45
(1,472)	1:122:B:THR:C	1:123:B:PHE:N	1:123:B:PHE:CA	1:123:B:PHE:C	4	1.45
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	8	1.44
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	12	1.44
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	8	1.44
(1,861)	1:64:D:VAL:N	1:64:D:VAL:CA	1:64:D:VAL:C	1:65:D:THR:N	14	1.44
(1,786)	1:23:D:PHE:C	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	17	1.44
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	13	1.44
(1,393)	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1:82:B:GLY:N	16	1.44
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	18	1.44
(1,303)	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	1:36:B:TRP:N	12	1.44
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	4	1.44
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	18	1.44
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	19	1.44
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	11	1.43
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	13	1.43
(1,603)	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	1:61:C:ARG:N	1	1.43
(1,552)	1:33:C:GLN:C	1:34:C:LYS:N	1:34:C:LYS:CA	1:34:C:LYS:C	18	1.43
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	7	1.43
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	3	1.43
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	8	1.43
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	15	1.43
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	2	1.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	16	1.43
(1,136)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	3	1.43
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	5	1.43
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	9	1.43
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	12	1.43
(1,66)	1:44:A:LEU:C	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	19	1.43
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	18	1.42
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	1	1.42
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	8	1.42
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	10	1.42
(1,223)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:ASN:N	14	1.42
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	8	1.42
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	16	1.42
(1,126)	1:74:A:PHE:C	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	12	1.42
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	16	1.42
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	6	1.41
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	20	1.41
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	20	1.41
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	6	1.41
(1,865)	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	1:67:D:SER:N	3	1.41
(1,652)	1:84:C:PHE:C	1:85:C:SER:N	1:85:C:SER:CA	1:85:C:SER:C	14	1.41
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	11	1.41
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	18	1.41
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	15	1.41
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	8	1.41
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1	1.41
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	16	1.41
(1,903)	1:85:D:SER:N	1:85:D:SER:CA	1:85:D:SER:C	1:86:D:ILE:N	9	1.4
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	6	1.4
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	11	1.4
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	10	1.4
(1,523)	1:17:C:TYR:N	1:17:C:TYR:CA	1:17:C:TYR:C	1:18:C:THR:N	19	1.4
(1,481)	1:128:B:LEU:N	1:128:B:LEU:CA	1:128:B:LEU:C	1:129:B:ALA:N	4	1.4
(1,385)	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	1:78:B:VAL:N	3	1.4
(1,352)	1:60:B:LEU:C	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	2	1.4
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	5	1.4
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	14	1.4
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	8	1.4
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	5	1.39
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	2	1.39
(1,799)	1:32:D:PHE:N	1:32:D:PHE:CA	1:32:D:PHE:C	1:33:D:GLN:N	18	1.39
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	10	1.39
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	5	1.39
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	7	1.39
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	9	1.39
(1,262)	1:12:B:GLN:C	1:13:B:ILE:N	1:13:B:ILE:CA	1:13:B:ILE:C	3	1.39
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	16	1.39
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	2	1.39
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	19	1.39
(1,61)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:ASP:N	3	1.39
(1,779)	1:20:D:ASP:N	1:20:D:ASP:CA	1:20:D:ASP:C	1:21:D:ILE:N	2	1.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,519)	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	1:16:C:ILE:N	7	1.38
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	13	1.38
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	5	1.38
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	3	1.38
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	18	1.38
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	3	1.37
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	12	1.37
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	16	1.37
(1,857)	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	1:63:D:THR:N	9	1.37
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	15	1.37
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	7	1.37
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	9	1.37
(1,571)	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	1:45:C:ASP:N	7	1.37
(1,519)	1:15:C:ARG:N	1:15:C:ARG:CA	1:15:C:ARG:C	1:16:C:ILE:N	18	1.37
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	2	1.37
(1,274)	1:18:B:THR:C	1:19:B:LYS:N	1:19:B:LYS:CA	1:19:B:LYS:C	7	1.37
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1	1.36
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	8	1.36
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	16	1.36
(1,581)	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	1:50:C:GLN:N	2	1.36
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	11	1.36
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	8	1.36
(1,370)	1:69:B:GLY:C	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	18	1.36
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	10	1.36
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	12	1.36
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	13	1.35
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	5	1.35
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	1	1.35
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	15	1.35
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	9	1.35
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	11	1.35
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	15	1.35
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	10	1.35
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	11	1.34
(1,872)	1:69:D:GLY:C	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	7	1.34
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	11	1.34
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	10	1.34
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	15	1.34
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	13	1.34
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	5	1.34
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	15	1.34
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	7	1.34
(1,128)	1:75:A:LEU:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	6	1.34
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	8	1.34
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	6	1.34
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	15	1.33
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	5	1.33
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	11	1.33
(1,612)	1:64:C:VAL:C	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	17	1.33
(1,593)	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	1:56:C:TYR:N	8	1.33
(1,513)	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	1:13:C:ILE:N	11	1.33

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	4	1.33
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	18	1.33
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	8	1.33
(1,287)	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	1:26:B:PRO:N	7	1.33
(1,263)	1:13:B:ILE:N	1:13:B:ILE:CA	1:13:B:ILE:C	1:14:B:GLN:N	5	1.33
(1,227)	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	1:129:A:ALA:N	19	1.33
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	7	1.33
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	11	1.33
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	5	1.33
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	6	1.32
(1,526)	1:18:C:THR:C	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	19	1.32
(1,118)	1:70:A:GLU:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	13	1.32
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	6	1.32
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	1	1.31
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	1	1.31
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	18	1.31
(1,787)	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	1:25:D:ALA:N	13	1.31
(1,671)	1:94:C:MET:N	1:94:C:MET:CA	1:94:C:MET:C	1:95:C:ALA:N	15	1.31
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	20	1.31
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	16	1.31
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	17	1.31
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	6	1.31
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	5	1.31
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	1	1.31
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	15	1.31
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	3	1.3
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	13	1.3
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	4	1.3
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	16	1.3
(1,504)	1:140:B:TYR:C	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	2	1.3
(1,481)	1:128:B:LEU:N	1:128:B:LEU:CA	1:128:B:LEU:C	1:129:B:ALA:N	15	1.3
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	17	1.3
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	13	1.3
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	9	1.3
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	14	1.3
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	3	1.3
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	4	1.3
(1,140)	1:81:A:GLY:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	4	1.3
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	9	1.3
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	12	1.3
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	7	1.3
(1,867)	1:67:D:SER:N	1:67:D:SER:CA	1:67:D:SER:C	1:68:D:LEU:N	17	1.29
(1,863)	1:65:D:THR:N	1:65:D:THR:CA	1:65:D:THR:C	1:66:D:ALA:N	14	1.29
(1,770)	1:15:D:ARG:C	1:16:D:ILE:N	1:16:D:ILE:CA	1:16:D:ILE:C	15	1.29
(1,723)	1:122:C:THR:N	1:122:C:THR:CA	1:122:C:THR:C	1:123:C:PHE:N	14	1.29
(1,626)	1:71:C:GLU:C	1:72:C:THR:N	1:72:C:THR:CA	1:72:C:THR:C	10	1.29
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	11	1.29
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	2	1.29
(1,222)	1:125:A:GLN:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	7	1.29
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	8	1.29
(1,67)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:THR:N	18	1.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1012)	1:143:D:GLN:C	1:144:D:GLN:N	1:144:D:GLN:CA	1:144:D:GLN:C	5	1.28
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	13	1.28
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	19	1.28
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	11	1.28
(1,803)	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	1:35:D:ASP:N	16	1.28
(1,709)	1:115:C:THR:N	1:115:C:THR:CA	1:115:C:THR:C	1:116:C:SER:N	17	1.28
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	15	1.28
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	11	1.28
(1,291)	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	1:29:B:PRO:N	14	1.28
(1,257)	1:10:B:THR:N	1:10:B:THR:CA	1:10:B:THR:C	1:11:B:PHE:N	4	1.28
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	2	1.28
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	2	1.28
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	16	1.28
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	16	1.28
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	8	1.27
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	20	1.27
(1,571)	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	1:45:C:ASP:N	3	1.27
(1,503)	1:140:B:TYR:N	1:140:B:TYR:CA	1:140:B:TYR:C	1:141:B:LEU:N	2	1.27
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	16	1.27
(1,393)	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1:82:B:GLY:N	2	1.27
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	3	1.27
(1,330)	1:49:B:SER:C	1:50:B:GLN:N	1:50:B:GLN:CA	1:50:B:GLN:C	8	1.27
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	4	1.27
(1,222)	1:125:A:GLN:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	6	1.27
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	18	1.27
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	13	1.27
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	10	1.27
(1,34)	1:26:A:PRO:C	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	19	1.27
(1,1012)	1:143:D:GLN:C	1:144:D:GLN:N	1:144:D:GLN:CA	1:144:D:GLN:C	14	1.26
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	17	1.26
(1,677)	1:97:C:CYS:N	1:97:C:CYS:CA	1:97:C:CYS:C	1:98:C:LEU:N	18	1.26
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	7	1.26
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	20	1.26
(1,497)	1:137:B:PHE:N	1:137:B:PHE:CA	1:137:B:PHE:C	1:138:B:MET:N	4	1.26
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	13	1.26
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	1	1.26
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	19	1.26
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	9	1.26
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	18	1.26
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	1	1.25
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	12	1.25
(1,647)	1:82:C:GLY:N	1:82:C:GLY:CA	1:82:C:GLY:C	1:83:C:ILE:N	7	1.25
(1,610)	1:63:C:THR:C	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	15	1.25
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	10	1.25
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	9	1.25
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	19	1.25
(1,306)	1:36:B:TRP:C	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	20	1.25
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	13	1.25
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	7	1.25
(1,35)	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1:28:A:ALA:N	12	1.25
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	9	1.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	2	1.24
(1,786)	1:23:D:PHE:C	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	15	1.24
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	7	1.24
(1,574)	1:45:C:ASP:C	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	10	1.24
(1,541)	1:27:C:ASN:N	1:27:C:ASN:CA	1:27:C:ASN:C	1:28:C:ALA:N	7	1.24
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	4	1.24
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	16	1.24
(1,481)	1:128:B:LEU:N	1:128:B:LEU:CA	1:128:B:LEU:C	1:129:B:ALA:N	5	1.24
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	7	1.24
(1,159)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:THR:N	15	1.24
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	15	1.24
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	6	1.24
(1,136)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	14	1.24
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	3	1.24
(1,128)	1:75:A:LEU:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	19	1.24
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	12	1.24
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	9	1.24
(1,51)	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	1:37:A:GLN:N	18	1.24
(1,44)	1:32:A:PHE:C	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	2	1.24
(1,893)	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	1:81:D:GLY:N	2	1.23
(1,887)	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	1:78:D:VAL:N	16	1.23
(1,872)	1:69:D:GLY:C	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	18	1.23
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	10	1.23
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	7	1.23
(1,395)	1:82:B:GLY:N	1:82:B:GLY:CA	1:82:B:GLY:C	1:83:B:ILE:N	7	1.23
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	12	1.23
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	19	1.23
(1,173)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:GLY:N	11	1.23
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	5	1.23
(1,80)	1:51:A:LEU:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	7	1.23
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	14	1.23
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	2	1.22
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	5	1.22
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	11	1.22
(1,848)	1:57:D:GLU:C	1:58:D:VAL:N	1:58:D:VAL:CA	1:58:D:VAL:C	20	1.22
(1,643)	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	1:81:C:GLY:N	2	1.22
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	2	1.22
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	19	1.22
(1,545)	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1:31:C:VAL:N	7	1.22
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	6	1.22
(1,373)	1:71:B:GLU:N	1:71:B:GLU:CA	1:71:B:GLU:C	1:72:B:THR:N	18	1.22
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	2	1.22
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	18	1.22
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	11	1.22
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	20	1.21
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	10	1.21
(1,826)	1:46:D:THR:C	1:47:D:ALA:N	1:47:D:ALA:CA	1:47:D:ALA:C	3	1.21
(1,659)	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	1:89:C:ILE:N	10	1.21
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	10	1.21
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	18	1.21
(1,510)	1:10:C:THR:C	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	14	1.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	10	1.21
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	16	1.21
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	10	1.21
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	17	1.21
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	7	1.21
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1	1.21
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	15	1.21
(1,320)	1:44:B:LEU:C	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	4	1.21
(1,128)	1:75:A:LEU:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	3	1.21
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	15	1.2
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	13	1.2
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	1	1.2
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	19	1.2
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	7	1.2
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	1	1.2
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	16	1.2
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	17	1.2
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	3	1.2
(1,128)	1:75:A:LEU:C	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1	1.2
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	7	1.2
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	4	1.19
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	7	1.19
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	20	1.19
(1,758)	1:9:D:MET:C	1:10:D:THR:N	1:10:D:THR:CA	1:10:D:THR:C	18	1.19
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	3	1.19
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	9	1.19
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	4	1.19
(1,424)	1:96:B:HIS:C	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	13	1.19
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	18	1.19
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	2	1.19
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	9	1.19
(1,938)	1:103:D:PRO:C	1:104:D:ASN:N	1:104:D:ASN:CA	1:104:D:ASN:C	2	1.18
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	13	1.18
(1,679)	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	1:99:C:GLY:N	6	1.18
(1,480)	1:127:B:ASN:C	1:128:B:LEU:N	1:128:B:LEU:CA	1:128:B:LEU:C	19	1.18
(1,469)	1:121:B:GLY:N	1:121:B:GLY:CA	1:121:B:GLY:C	1:122:B:THR:N	19	1.18
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	13	1.18
(1,214)	1:120:A:ARG:C	1:121:A:GLY:N	1:121:A:GLY:CA	1:121:A:GLY:C	12	1.18
(1,173)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:GLY:N	14	1.18
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	12	1.18
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	17	1.17
(1,173)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:GLY:N	12	1.17
(1,140)	1:81:A:GLY:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	12	1.17
(1,876)	1:71:D:GLU:C	1:72:D:THR:N	1:72:D:THR:CA	1:72:D:THR:C	3	1.16
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	20	1.16
(1,673)	1:95:C:ALA:N	1:95:C:ALA:CA	1:95:C:ALA:C	1:96:C:HIS:N	8	1.16
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	19	1.16
(1,606)	1:61:C:ARG:C	1:62:C:VAL:N	1:62:C:VAL:CA	1:62:C:VAL:C	10	1.16
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	14	1.16
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	17	1.16
(1,367)	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	1:69:B:GLY:N	6	1.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	13	1.16
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	13	1.16
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	19	1.15
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	14	1.15
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	6	1.15
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	17	1.15
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	4	1.15
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	18	1.15
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	4	1.15
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	16	1.15
(1,290)	1:27:B:ASN:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	17	1.15
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	5	1.15
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	10	1.15
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	9	1.15
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	9	1.14
(1,976)	1:124:D:PRO:C	1:125:D:GLN:N	1:125:D:GLN:CA	1:125:D:GLN:C	2	1.14
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	6	1.14
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	7	1.14
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	17	1.14
(1,554)	1:34:C:LYS:C	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	6	1.14
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	5	1.14
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	15	1.14
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	4	1.14
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	14	1.14
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	7	1.14
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	11	1.13
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	16	1.13
(1,822)	1:44:D:LEU:C	1:45:D:ASP:N	1:45:D:ASP:CA	1:45:D:ASP:C	18	1.13
(1,791)	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	1:28:D:ALA:N	4	1.13
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	12	1.13
(1,738)	1:131:C:VAL:C	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	5	1.13
(1,728)	1:125:C:GLN:C	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	18	1.13
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	17	1.13
(1,400)	1:84:B:PHE:C	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	8	1.13
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	16	1.13
(1,303)	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	1:36:B:TRP:N	11	1.13
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	3	1.13
(1,146)	1:84:A:PHE:C	1:85:A:SER:N	1:85:A:SER:CA	1:85:A:SER:C	16	1.13
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	3	1.13
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	16	1.12
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	10	1.12
(1,661)	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	1:90:C:GLU:N	17	1.12
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	14	1.12
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	7	1.12
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	3	1.12
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	11	1.12
(1,307)	1:37:B:GLN:N	1:37:B:GLN:CA	1:37:B:GLN:C	1:38:B:PRO:N	17	1.12
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1	1.12
(1,264)	1:13:B:ILE:C	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	4	1.12
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	1	1.12
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	5	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1	1.12
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	1	1.11
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	14	1.11
(1,659)	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	1:89:C:ILE:N	1	1.11
(1,648)	1:82:C:GLY:C	1:83:C:ILE:N	1:83:C:ILE:CA	1:83:C:ILE:C	8	1.11
(1,619)	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1:69:C:GLY:N	16	1.11
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	6	1.11
(1,516)	1:13:C:ILE:C	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	13	1.11
(1,471)	1:122:B:THR:N	1:122:B:THR:CA	1:122:B:THR:C	1:123:B:PHE:N	10	1.11
(1,414)	1:91:B:GLY:C	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	16	1.11
(1,403)	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1:87:B:ALA:N	9	1.11
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	2	1.11
(1,350)	1:59:B:VAL:C	1:60:B:LEU:N	1:60:B:LEU:CA	1:60:B:LEU:C	16	1.11
(1,249)	1:140:A:TYR:N	1:140:A:TYR:CA	1:140:A:TYR:C	1:141:A:LEU:N	15	1.11
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	11	1.11
(1,32)	1:24:A:GLU:C	1:25:A:ALA:N	1:25:A:ALA:CA	1:25:A:ALA:C	8	1.11
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	6	1.11
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	13	1.1
(1,749)	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	1:138:C:MET:N	16	1.1
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	7	1.1
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	15	1.1
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	8	1.1
(1,453)	1:113:B:CYS:N	1:113:B:CYS:CA	1:113:B:CYS:C	1:114:B:ILE:N	18	1.1
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	1	1.1
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	4	1.1
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	10	1.1
(1,290)	1:27:B:ASN:C	1:28:B:ALA:N	1:28:B:ALA:CA	1:28:B:ALA:C	9	1.1
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	1	1.1
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	2	1.09
(1,616)	1:66:C:ALA:C	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	3	1.09
(1,616)	1:66:C:ALA:C	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	4	1.09
(1,472)	1:122:B:THR:C	1:123:B:PHE:N	1:123:B:PHE:CA	1:123:B:PHE:C	10	1.09
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	12	1.09
(1,106)	1:64:A:VAL:C	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	5	1.09
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	13	1.09
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	3	1.08
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	6	1.08
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	19	1.08
(1,820)	1:43:D:ASP:C	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	13	1.08
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	4	1.08
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	18	1.08
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	13	1.08
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	16	1.08
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	4	1.08
(1,472)	1:122:B:THR:C	1:123:B:PHE:N	1:123:B:PHE:CA	1:123:B:PHE:C	5	1.08
(1,414)	1:91:B:GLY:C	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	12	1.08
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	2	1.08
(1,258)	1:10:B:THR:C	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	11	1.08
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	17	1.08
(1,136)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	19	1.08
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	16	1.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	18	1.08
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	17	1.07
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	5	1.07
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	6	1.07
(1,352)	1:60:B:LEU:C	1:61:B:ARG:N	1:61:B:ARG:CA	1:61:B:ARG:C	12	1.07
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	2	1.07
(1,915)	1:91:D:GLY:N	1:91:D:GLY:CA	1:91:D:GLY:C	1:92:D:THR:N	17	1.06
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	17	1.06
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	8	1.06
(1,324)	1:46:B:THR:C	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	14	1.06
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	19	1.06
(1,34)	1:26:A:PRO:C	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	1	1.06
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	15	1.05
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	11	1.05
(1,348)	1:58:B:VAL:C	1:59:B:VAL:N	1:59:B:VAL:CA	1:59:B:VAL:C	13	1.05
(1,301)	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	1:35:B:ASP:N	3	1.05
(1,272)	1:17:B:TYR:C	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	12	1.05
(1,181)	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	1:103:A:PRO:N	13	1.05
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	3	1.05
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	13	1.05
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	3	1.04
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	17	1.04
(1,856)	1:61:D:ARG:C	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	5	1.04
(1,825)	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1:47:D:ALA:N	18	1.04
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	3	1.04
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	8	1.04
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	18	1.04
(1,739)	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	1:133:C:PHE:N	13	1.04
(1,604)	1:60:C:LEU:C	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	10	1.04
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	13	1.04
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	8	1.04
(1,472)	1:122:B:THR:C	1:123:B:PHE:N	1:123:B:PHE:CA	1:123:B:PHE:C	2	1.04
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	18	1.04
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	10	1.04
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	13	1.04
(1,800)	1:32:D:PHE:C	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	2	1.03
(1,510)	1:10:C:THR:C	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	16	1.03
(1,383)	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	1:77:B:GLU:N	6	1.03
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	10	1.03
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	18	1.03
(1,79)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	17	1.03
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	2	1.02
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	19	1.02
(1,788)	1:24:D:GLU:C	1:25:D:ALA:N	1:25:D:ALA:CA	1:25:D:ALA:C	1	1.02
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	13	1.02
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	18	1.02
(1,648)	1:82:C:GLY:C	1:83:C:ILE:N	1:83:C:ILE:CA	1:83:C:ILE:C	2	1.02
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	2	1.02
(1,635)	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1:77:C:GLU:N	9	1.02
(1,606)	1:61:C:ARG:C	1:62:C:VAL:N	1:62:C:VAL:CA	1:62:C:VAL:C	7	1.02
(1,429)	1:99:B:GLY:N	1:99:B:GLY:CA	1:99:B:GLY:C	1:100:B:ALA:N	12	1.02

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	16	1.02
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	10	1.02
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	20	1.02
(1,29)	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	1:24:A:GLU:N	14	1.02
(1,835)	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	1:52:D:ALA:N	14	1.01
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	8	1.01
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	8	1.01
(1,599)	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	1:59:C:VAL:N	18	1.01
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	8	1.01
(1,517)	1:14:C:GLN:N	1:14:C:GLN:CA	1:14:C:GLN:C	1:15:C:ARG:N	17	1.01
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	7	1.01
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	10	1.01
(1,130)	1:76:A:CYS:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	19	1.01
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	6	1.0
(1,828)	1:47:D:ALA:C	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	14	1.0
(1,783)	1:22:D:SER:N	1:22:D:SER:CA	1:22:D:SER:C	1:23:D:PHE:N	8	1.0
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	2	1.0