Full wwPDB NMR Structure Validation Report (i)

Mar 25, 2026 – 09:02 AM UTC

PDB ID	:	5JTP / pdb_00005jtp
BMRB ID	:	30084
Title	:	The structure of chaperone SecB in complex with unstructured proPhoA binding site e
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

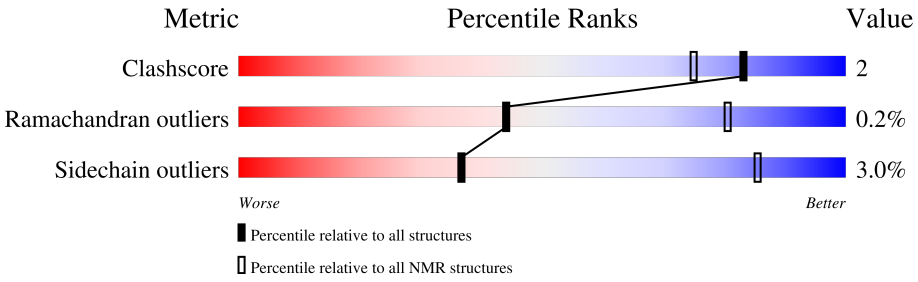
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 14%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	155	81% · 17%
1	B	155	79% · 17%
1	C	155	77% 5% · 17%
1	D	155	80% · 17%
2	E	22	100%
2	F	22	100%
2	G	22	100%
2	H	22	100%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:138, B:10-B:137, C:10-C:137, D:10-D:137 (513)	0.79	15

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 6 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10844 atoms, of which 5324 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	22	Total	C	H	N	O	S	0
			344	108	176	26	33	1	
2	F	22	Total	C	H	N	O	S	0
			344	108	176	26	33	1	
2	G	22	Total	C	H	N	O	S	0
			344	108	176	26	33	1	
2	H	22	Total	C	H	N	O	S	0
			344	108	176	26	33	1	

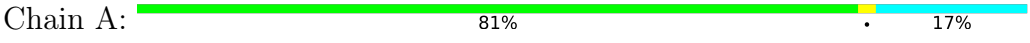
4 Residue-property plots

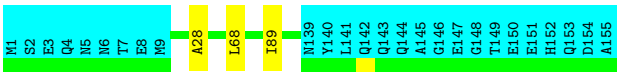
4.1 Average score per residue in the NMR ensemble

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

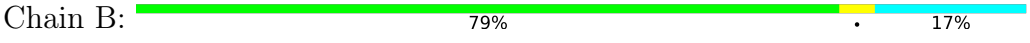
Chain A:

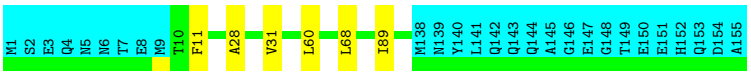




• Molecule 1: Protein-export protein SecB

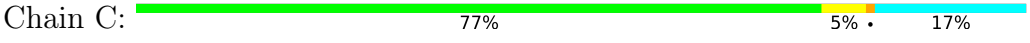
Chain B:





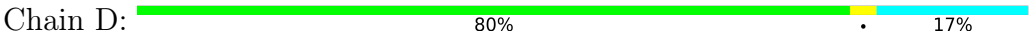
• Molecule 1: Protein-export protein SecB

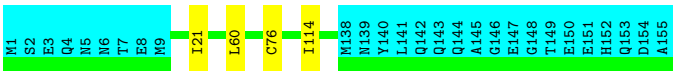
Chain C:



• Molecule 1: Protein-export protein SecB

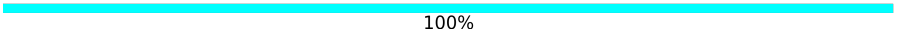
Chain D:





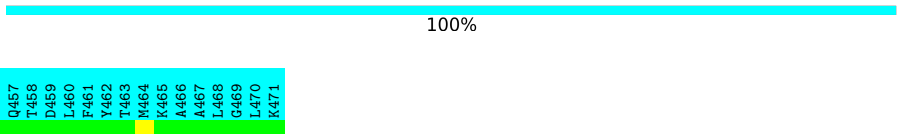
• Molecule 2: Alkaline phosphatase

Chain E:



• Molecule 2: Alkaline phosphatase

Chain F:

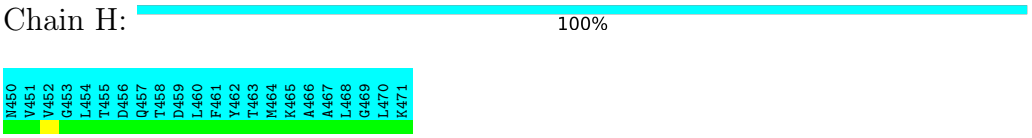


• Molecule 2: Alkaline phosphatase

Chain G:

• Molecule 2: Alkaline phosphatase

Chain H:



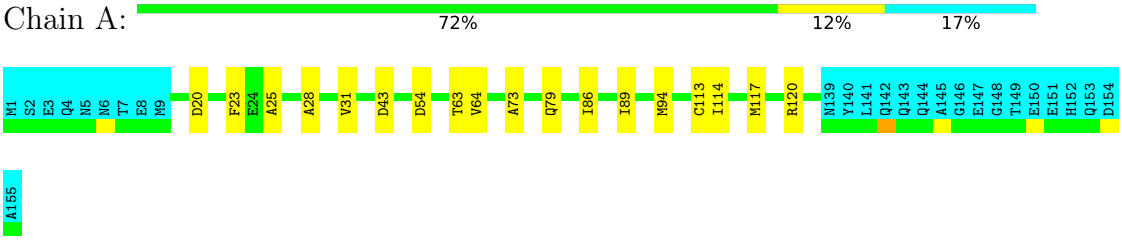
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

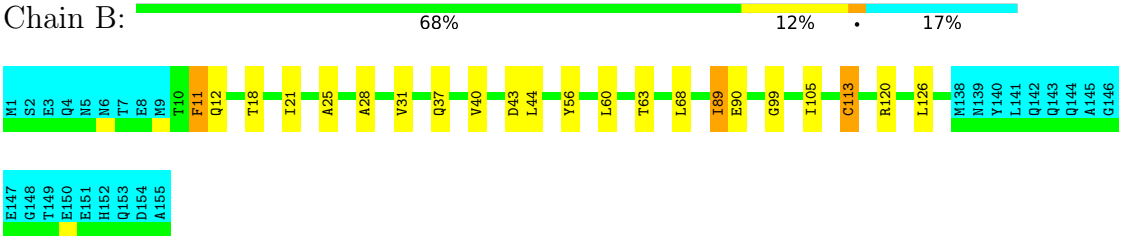
• Molecule 1: Protein-export protein SecB

Chain A:



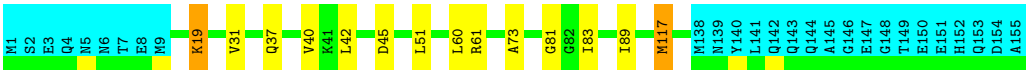
• Molecule 1: Protein-export protein SecB

Chain B:



• Molecule 1: Protein-export protein SecB

Chain C:

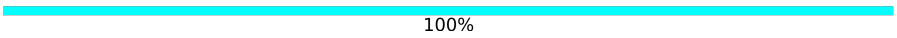


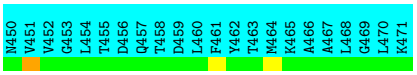
• Molecule 1: Protein-export protein SecB

Chain D:

• Molecule 2: Alkaline phosphatase

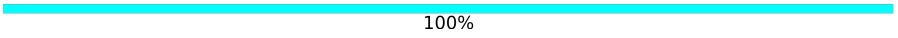
Chain E:





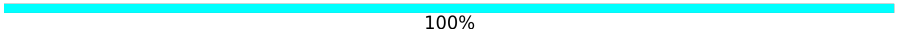
• Molecule 2: Alkaline phosphatase

Chain F:



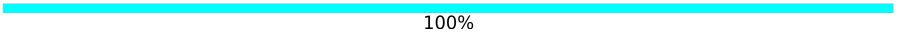
• Molecule 2: Alkaline phosphatase

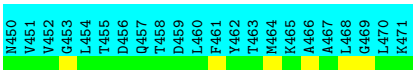
Chain G:



• Molecule 2: Alkaline phosphatase

Chain H:





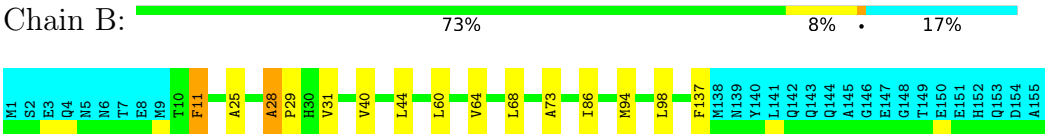
4.2.2 Score per residue for model 2

• Molecule 1: Protein-export protein SecB

Chain A:

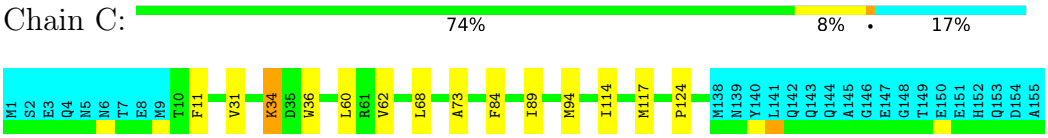
• Molecule 1: Protein-export protein SecB

Chain B:



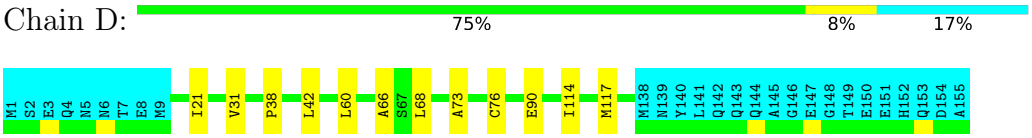
• Molecule 1: Protein-export protein SecB

Chain C:



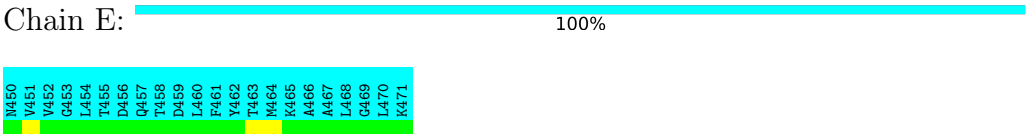
• Molecule 1: Protein-export protein SecB

Chain D:



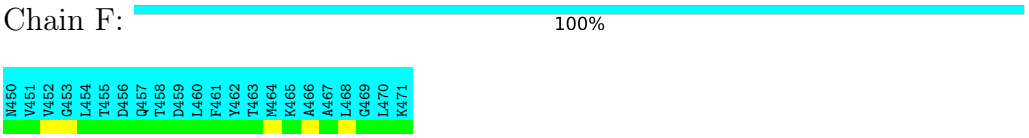
• Molecule 2: Alkaline phosphatase

Chain E:



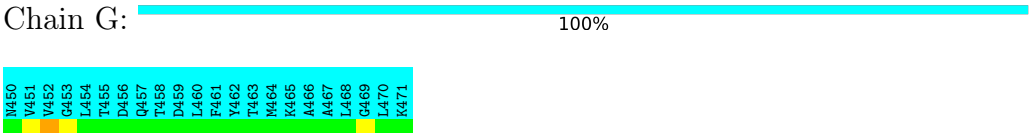
• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:



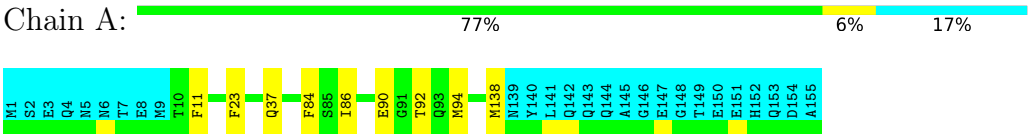
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.3 Score per residue for model 3

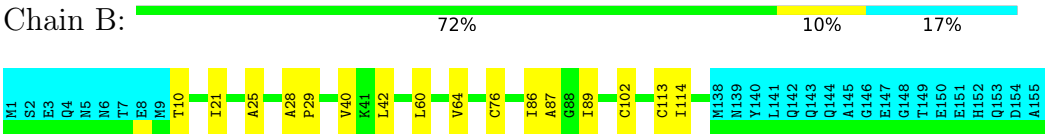
• Molecule 1: Protein-export protein SecB

Chain A:



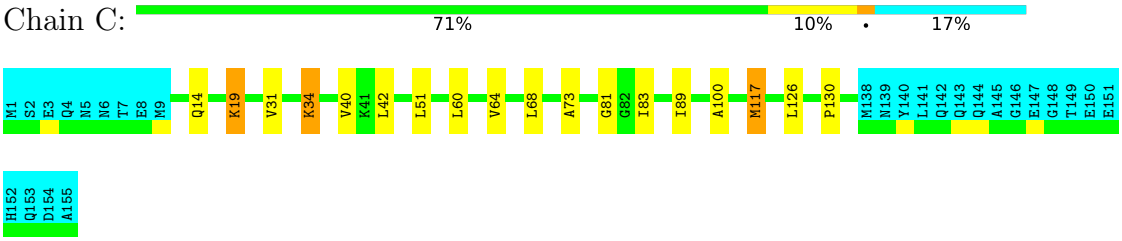
• Molecule 1: Protein-export protein SecB

Chain B:



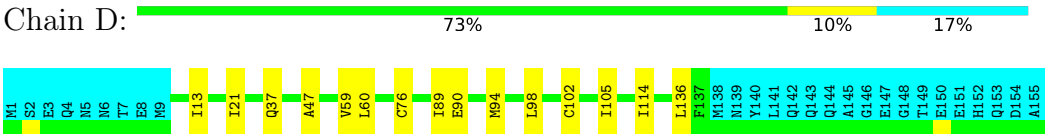
• Molecule 1: Protein-export protein SecB

Chain C:



• Molecule 1: Protein-export protein SecB

Chain D:

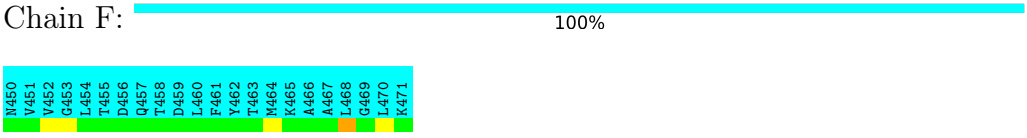


• Molecule 2: Alkaline phosphatase

Chain E:

• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:

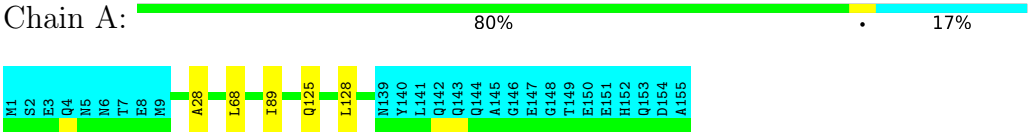
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.4 Score per residue for model 4

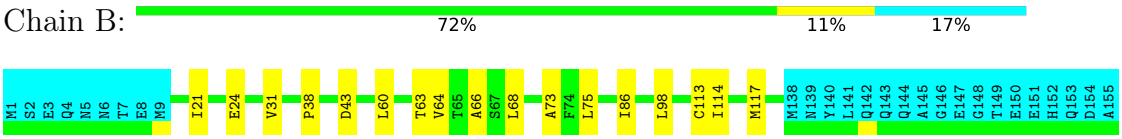
• Molecule 1: Protein-export protein SecB

Chain A:



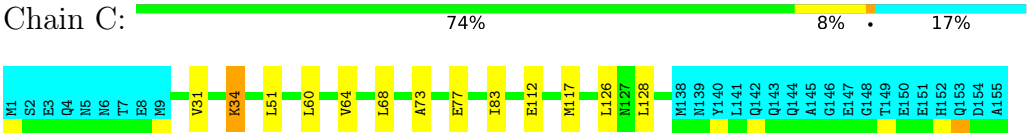
• Molecule 1: Protein-export protein SecB

Chain B:



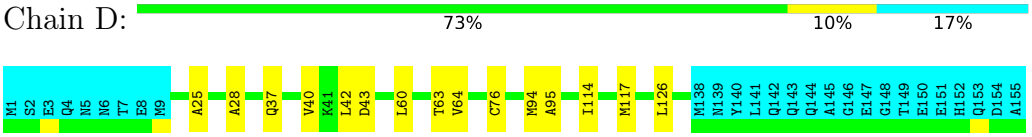
• Molecule 1: Protein-export protein SecB

Chain C:



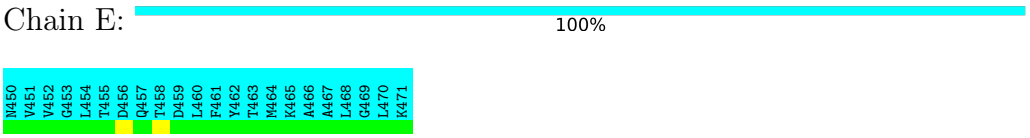
• Molecule 1: Protein-export protein SecB

Chain D:



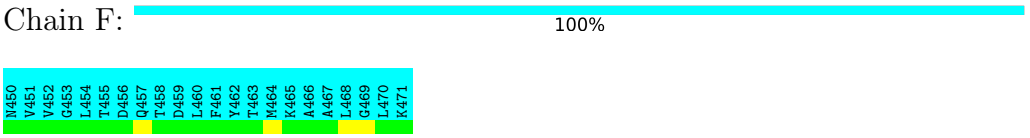
• Molecule 2: Alkaline phosphatase

Chain E:



• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:

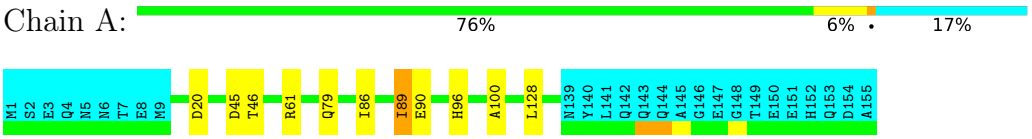
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.5 Score per residue for model 5

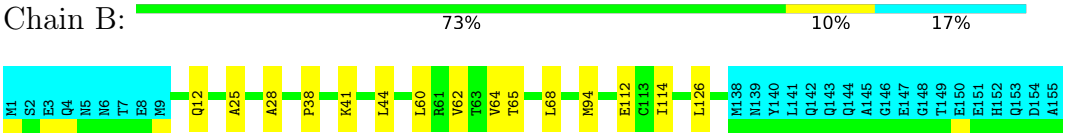
• Molecule 1: Protein-export protein SecB

Chain A:



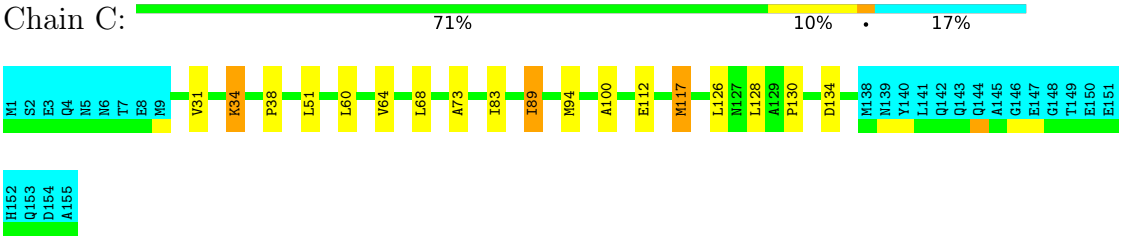
• Molecule 1: Protein-export protein SecB

Chain B:



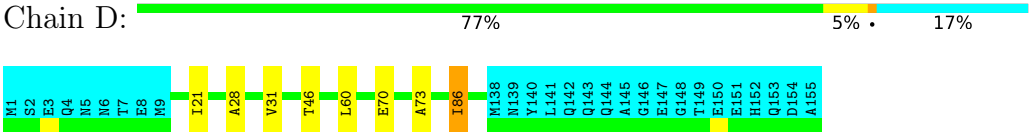
• Molecule 1: Protein-export protein SecB

Chain C:



• Molecule 1: Protein-export protein SecB

Chain D:

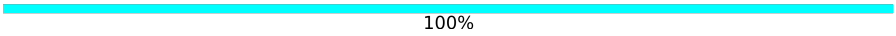


• Molecule 2: Alkaline phosphatase

Chain E:

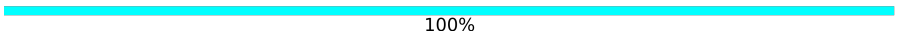
• Molecule 2: Alkaline phosphatase

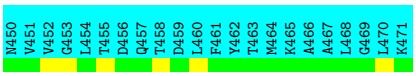
Chain F:



• Molecule 2: Alkaline phosphatase

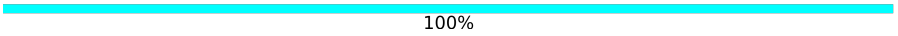
Chain G:





• Molecule 2: Alkaline phosphatase

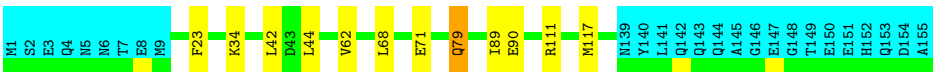
Chain H:



4.2.6 Score per residue for model 6

• Molecule 1: Protein-export protein SecB

Chain A:



• Molecule 1: Protein-export protein SecB

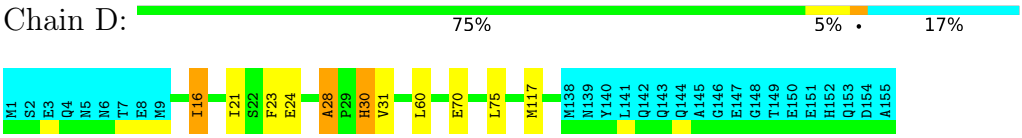
Chain B:

• Molecule 1: Protein-export protein SecB

Chain C:

• Molecule 1: Protein-export protein SecB

Chain D:

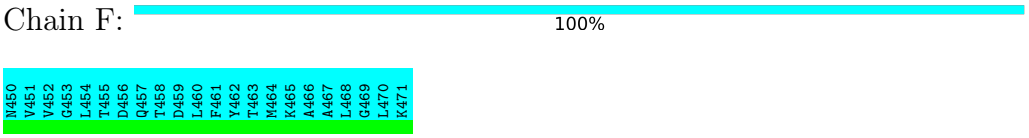


• Molecule 2: Alkaline phosphatase

Chain E:

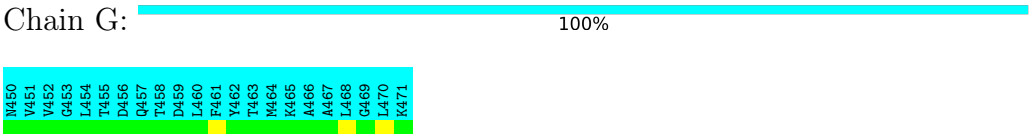
• Molecule 2: Alkaline phosphatase

Chain F:



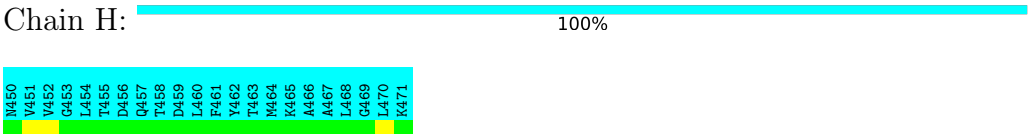
• Molecule 2: Alkaline phosphatase

Chain G:



• Molecule 2: Alkaline phosphatase

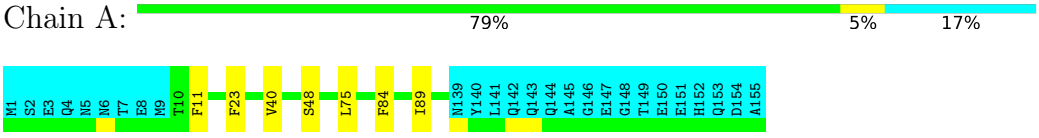
Chain H:



4.2.7 Score per residue for model 7

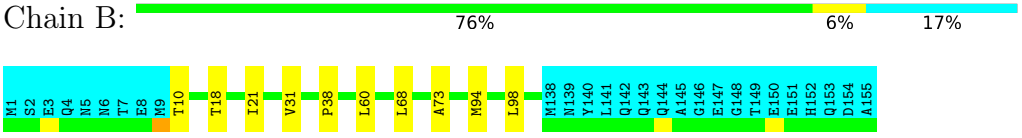
• Molecule 1: Protein-export protein SecB

Chain A:



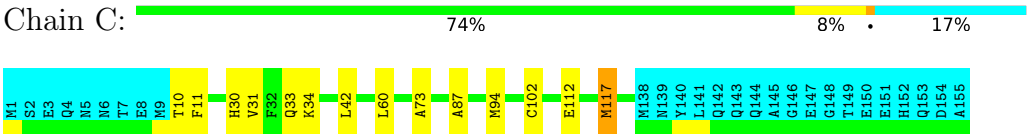
• Molecule 1: Protein-export protein SecB

Chain B:



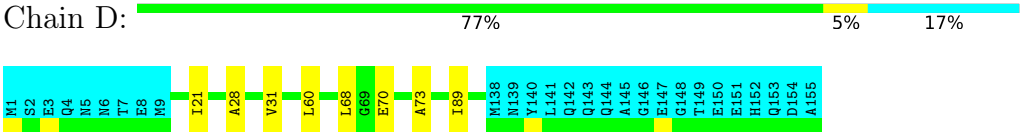
• Molecule 1: Protein-export protein SecB

Chain C:



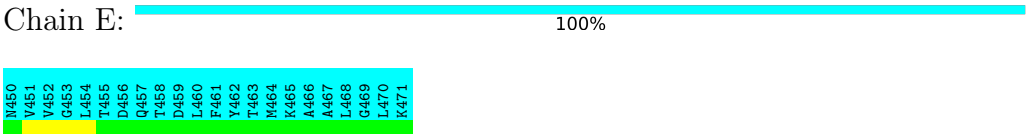
• Molecule 1: Protein-export protein SecB

Chain D:



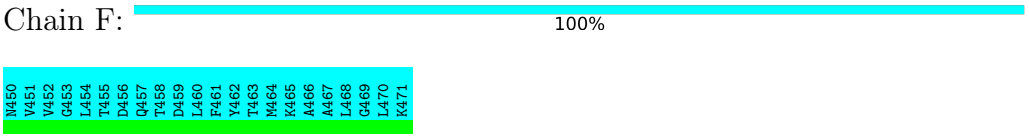
• Molecule 2: Alkaline phosphatase

Chain E:



• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:

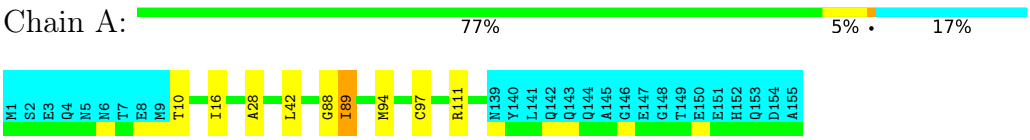
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.8 Score per residue for model 8

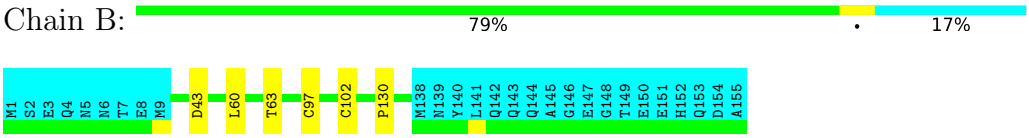
• Molecule 1: Protein-export protein SecB

Chain A:



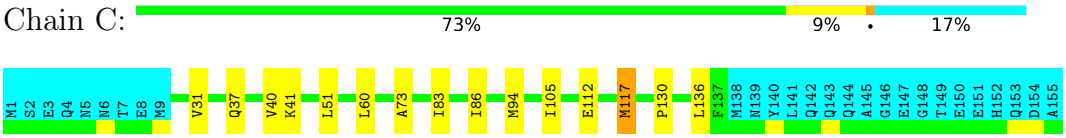
• Molecule 1: Protein-export protein SecB

Chain B:



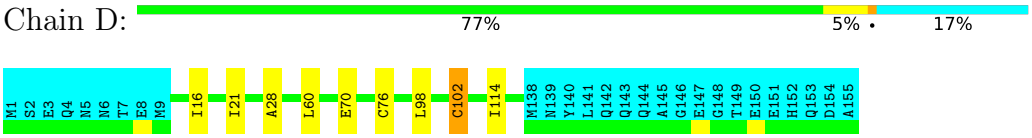
• Molecule 1: Protein-export protein SecB

Chain C:



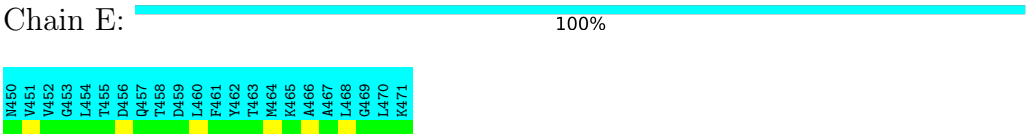
• Molecule 1: Protein-export protein SecB

Chain D:



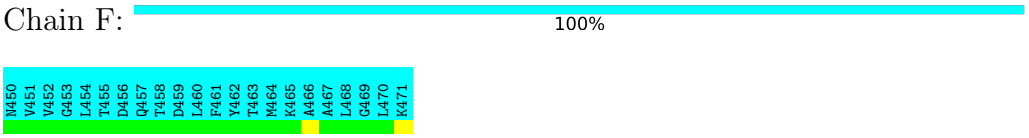
• Molecule 2: Alkaline phosphatase

Chain E:



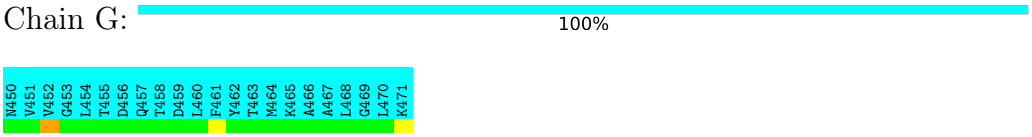
• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:



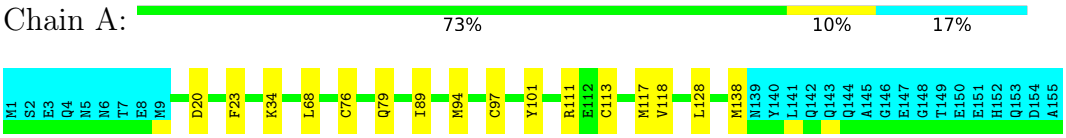
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.9 Score per residue for model 9

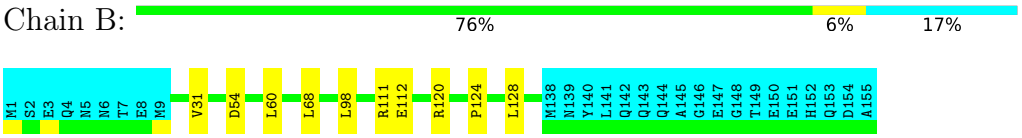
• Molecule 1: Protein-export protein SecB

Chain A:



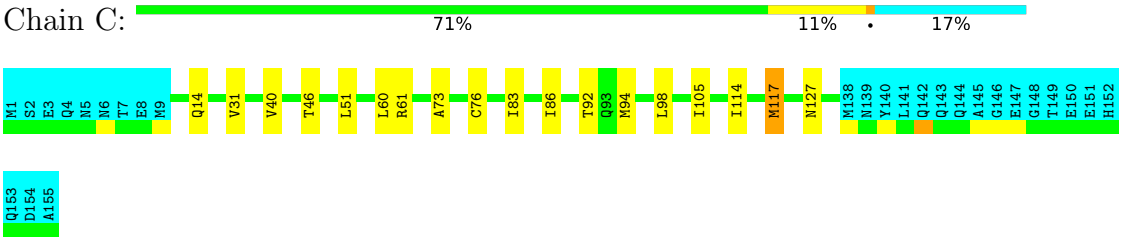
• Molecule 1: Protein-export protein SecB

Chain B:



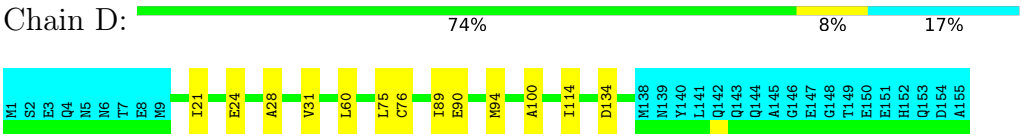
• Molecule 1: Protein-export protein SecB

Chain C:



• Molecule 1: Protein-export protein SecB

Chain D:

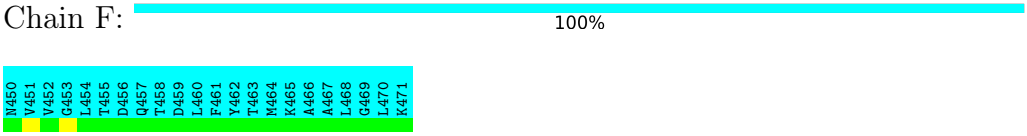


• Molecule 2: Alkaline phosphatase

Chain E:

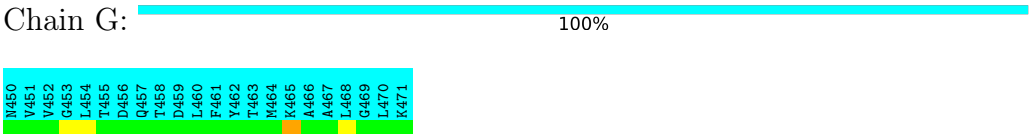
• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:



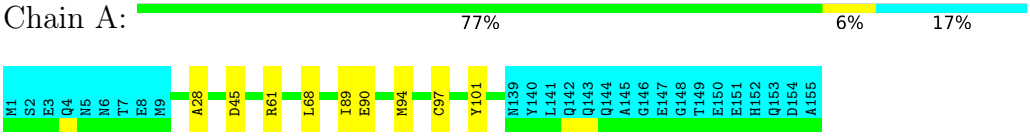
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.10 Score per residue for model 10

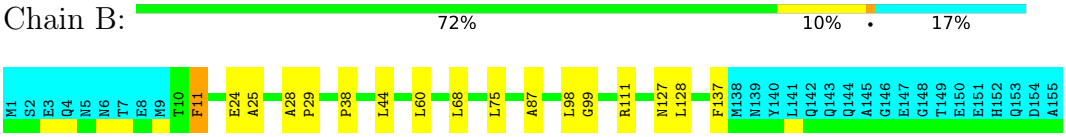
• Molecule 1: Protein-export protein SecB

Chain A:



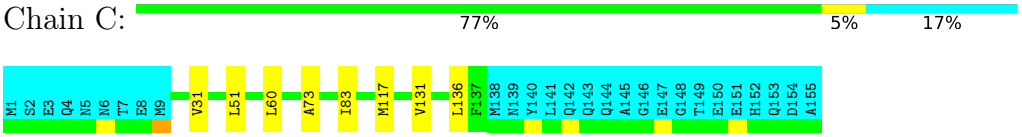
• Molecule 1: Protein-export protein SecB

Chain B:



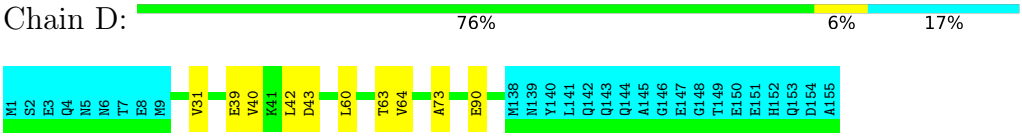
• Molecule 1: Protein-export protein SecB

Chain C:



• Molecule 1: Protein-export protein SecB

Chain D:



• Molecule 2: Alkaline phosphatase

Chain E:

• Molecule 2: Alkaline phosphatase

Chain F:

• Molecule 2: Alkaline phosphatase

Chain G:

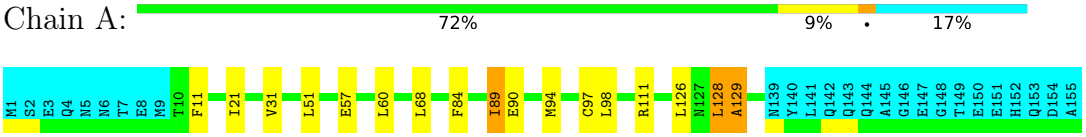
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.11 Score per residue for model 11

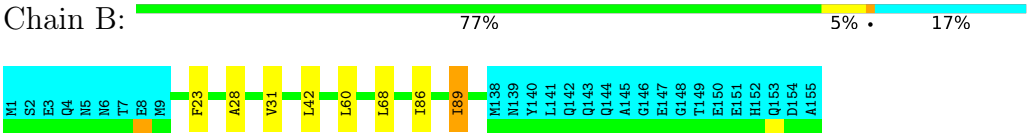
• Molecule 1: Protein-export protein SecB

Chain A:



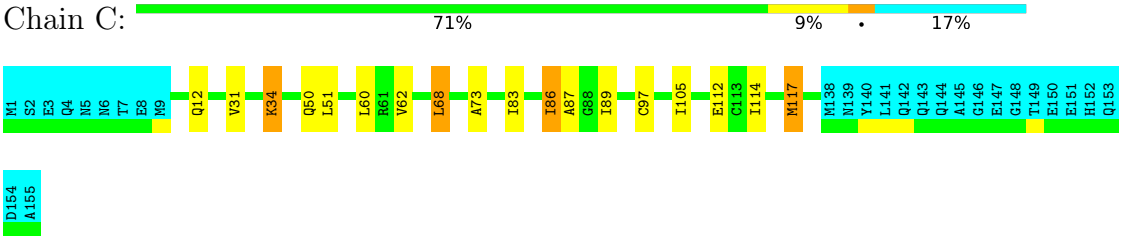
• Molecule 1: Protein-export protein SecB

Chain B:



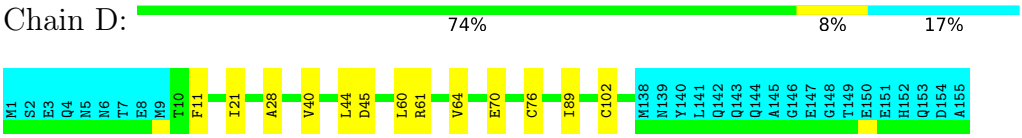
• Molecule 1: Protein-export protein SecB

Chain C:



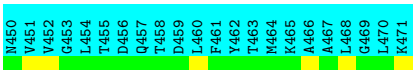
• Molecule 1: Protein-export protein SecB

Chain D:



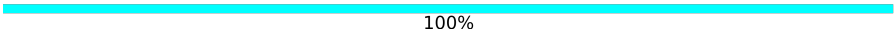
• Molecule 2: Alkaline phosphatase

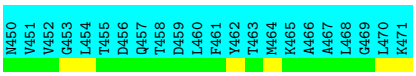
Chain E:



• Molecule 2: Alkaline phosphatase

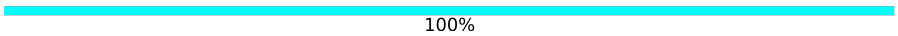
Chain F:

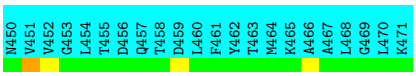




• Molecule 2: Alkaline phosphatase

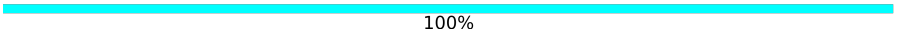
Chain G:

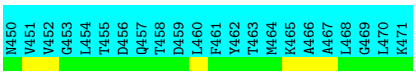




• Molecule 2: Alkaline phosphatase

Chain H:

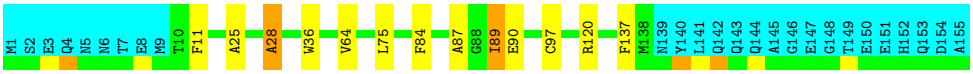




4.2.12 Score per residue for model 12

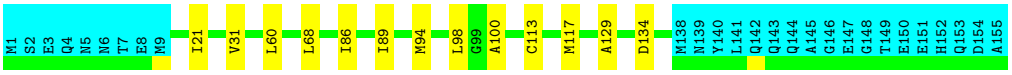
• Molecule 1: Protein-export protein SecB

Chain A:



• Molecule 1: Protein-export protein SecB

Chain B:

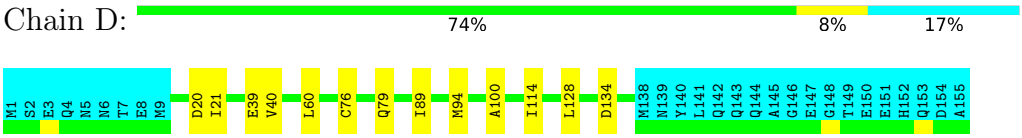


• Molecule 1: Protein-export protein SecB

Chain C:

• Molecule 1: Protein-export protein SecB

Chain D:

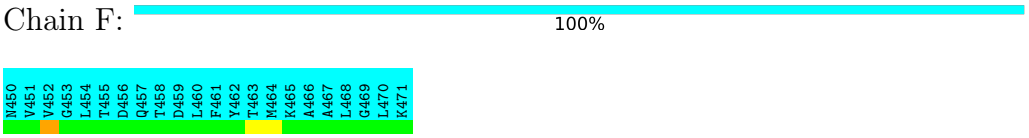


• Molecule 2: Alkaline phosphatase

Chain E:

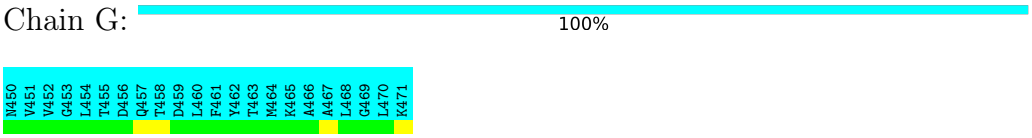
• Molecule 2: Alkaline phosphatase

Chain F:



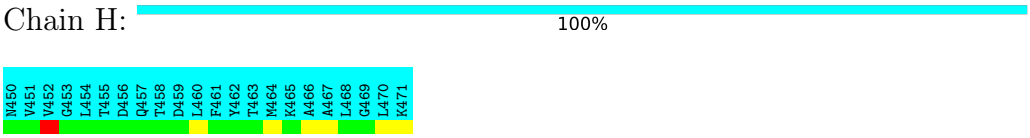
• Molecule 2: Alkaline phosphatase

Chain G:



• Molecule 2: Alkaline phosphatase

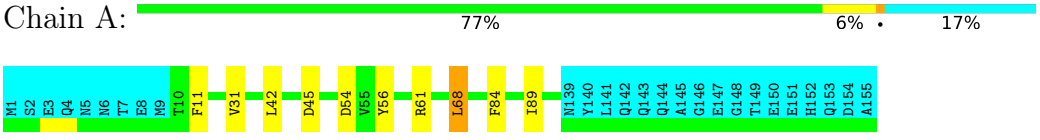
Chain H:



4.2.13 Score per residue for model 13

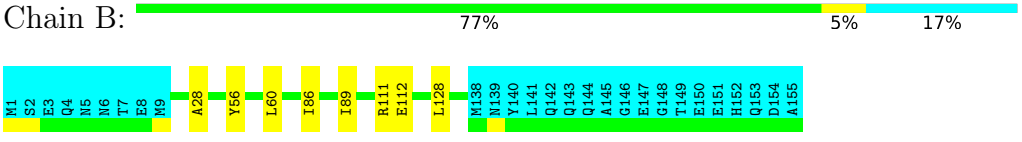
• Molecule 1: Protein-export protein SecB

Chain A:



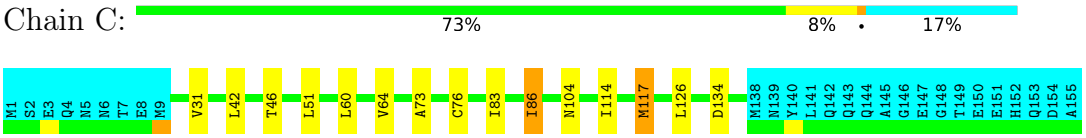
• Molecule 1: Protein-export protein SecB

Chain B:



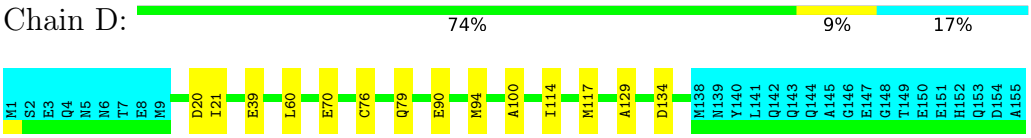
• Molecule 1: Protein-export protein SecB

Chain C:



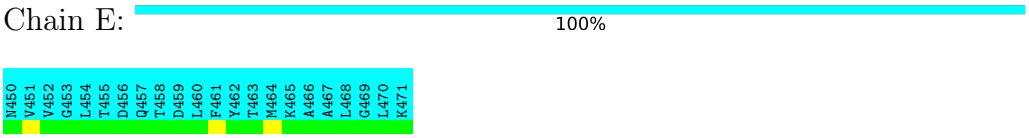
• Molecule 1: Protein-export protein SecB

Chain D:



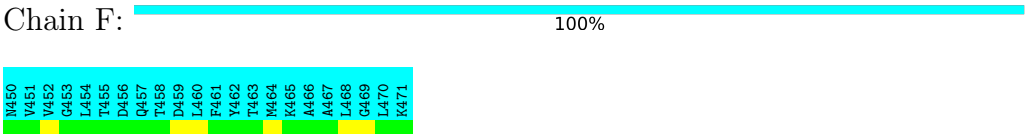
• Molecule 2: Alkaline phosphatase

Chain E:



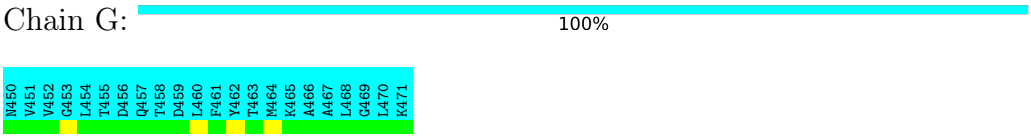
• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:



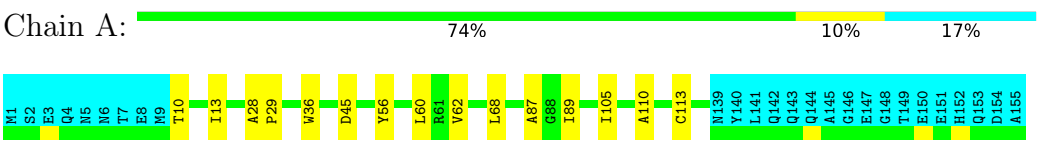
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.14 Score per residue for model 14

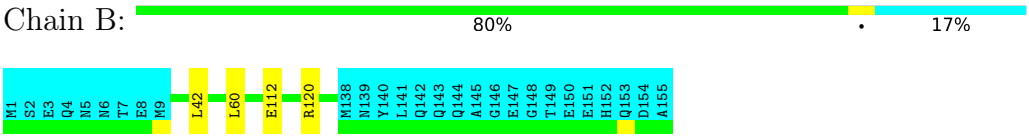
• Molecule 1: Protein-export protein SecB

Chain A:



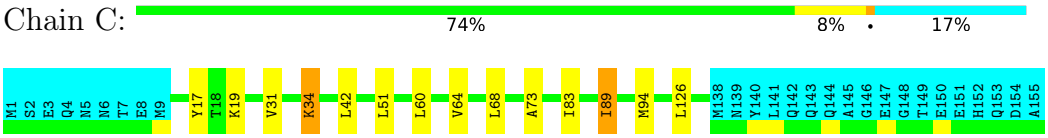
• Molecule 1: Protein-export protein SecB

Chain B:



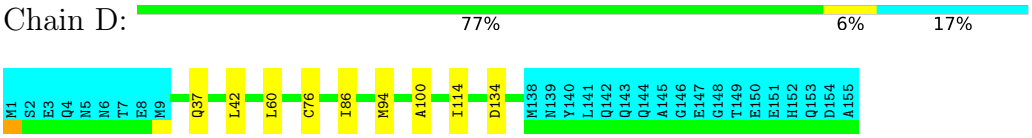
• Molecule 1: Protein-export protein SecB

Chain C:



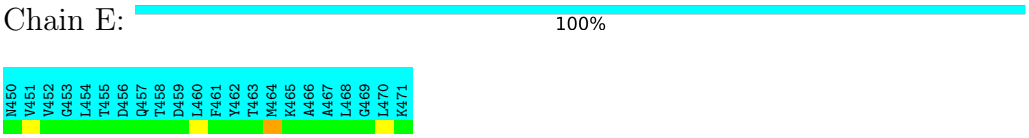
• Molecule 1: Protein-export protein SecB

Chain D:



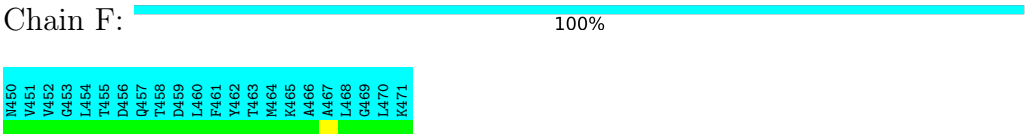
• Molecule 2: Alkaline phosphatase

Chain E:



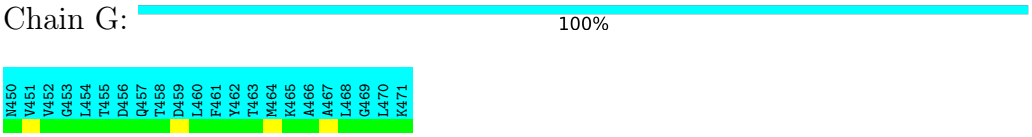
• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:



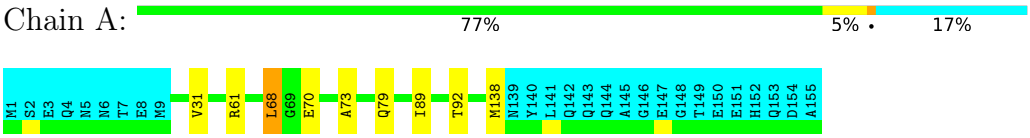
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.15 Score per residue for model 15 (medoid)

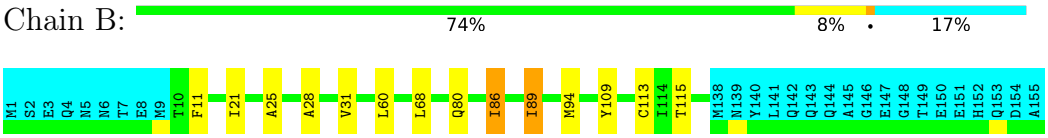
• Molecule 1: Protein-export protein SecB

Chain A:



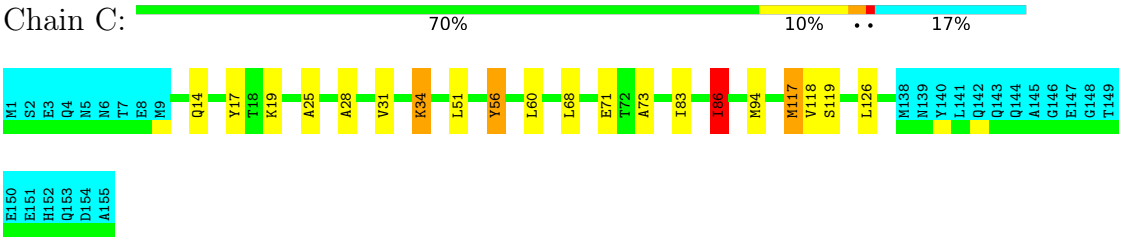
• Molecule 1: Protein-export protein SecB

Chain B:



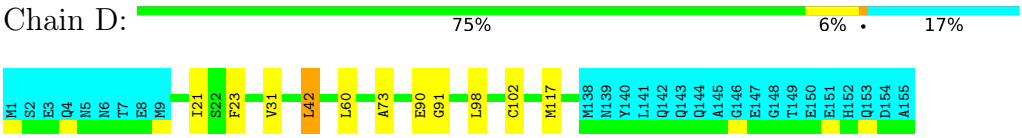
• Molecule 1: Protein-export protein SecB

Chain C:



• Molecule 1: Protein-export protein SecB

Chain D:

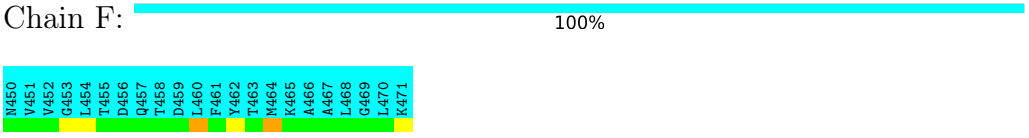


• Molecule 2: Alkaline phosphatase

Chain E:

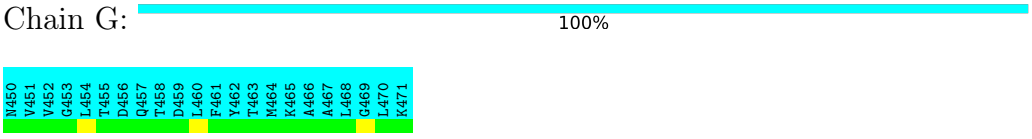
• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:



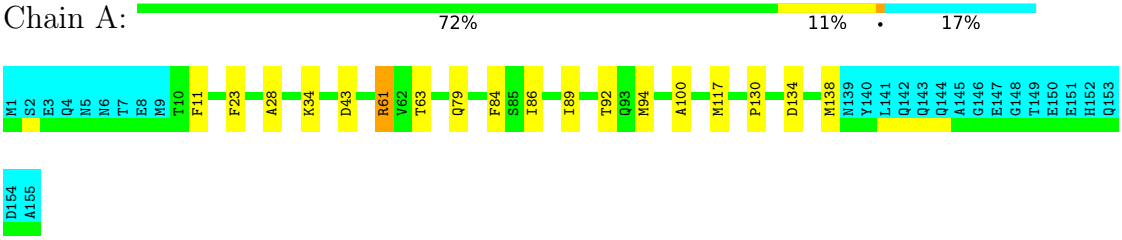
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.16 Score per residue for model 16

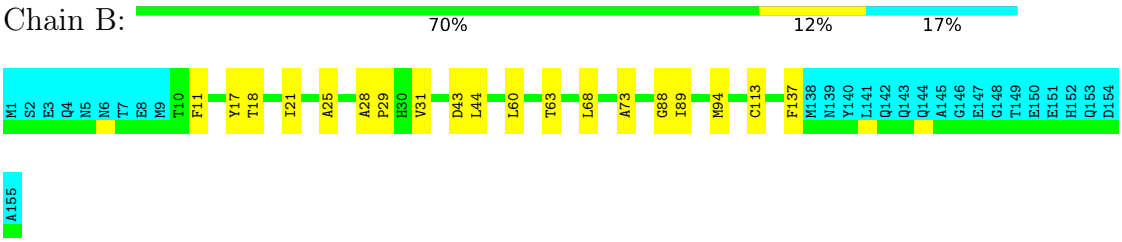
• Molecule 1: Protein-export protein SecB

Chain A:



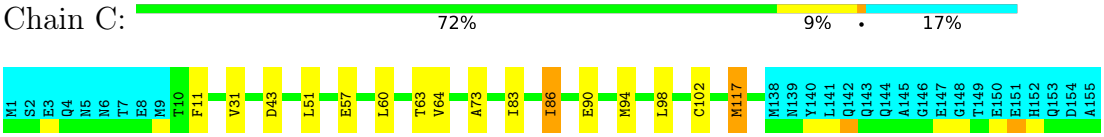
• Molecule 1: Protein-export protein SecB

Chain B:



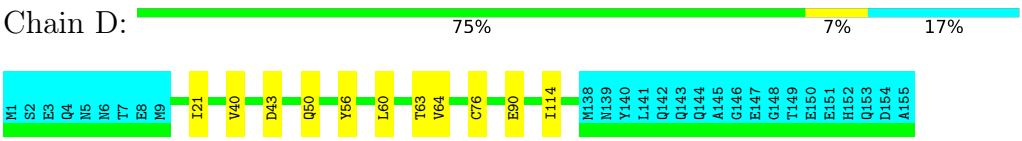
• Molecule 1: Protein-export protein SecB

Chain C:



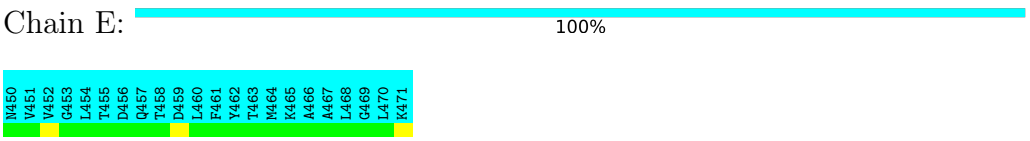
• Molecule 1: Protein-export protein SecB

Chain D:



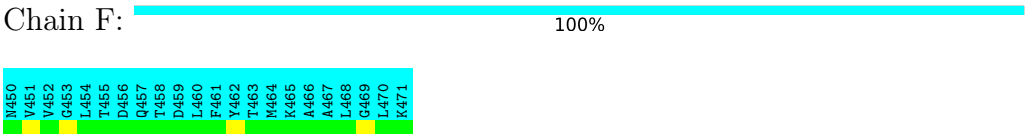
• Molecule 2: Alkaline phosphatase

Chain E:



• Molecule 2: Alkaline phosphatase

Chain F:

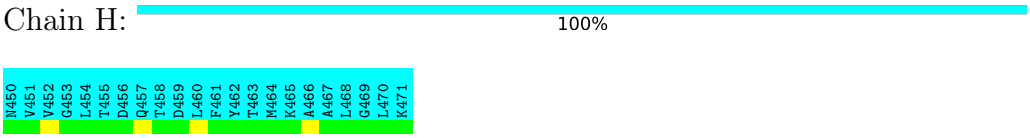


• Molecule 2: Alkaline phosphatase

Chain G:

• Molecule 2: Alkaline phosphatase

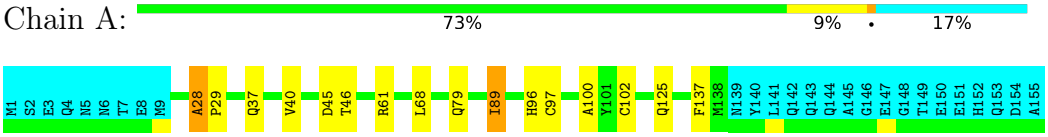
Chain H:



4.2.17 Score per residue for model 17

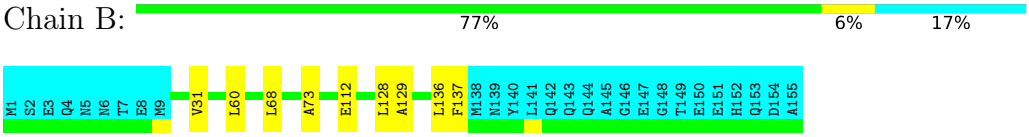
• Molecule 1: Protein-export protein SecB

Chain A:



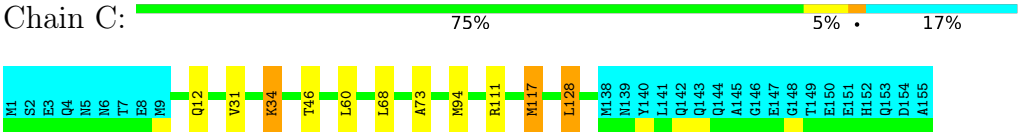
• Molecule 1: Protein-export protein SecB

Chain B:



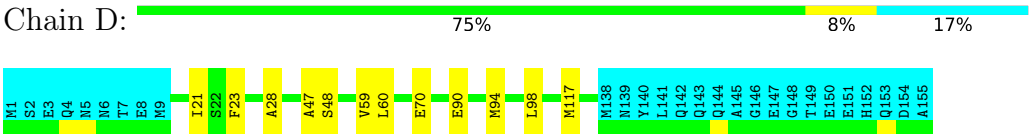
• Molecule 1: Protein-export protein SecB

Chain C:



• Molecule 1: Protein-export protein SecB

Chain D:

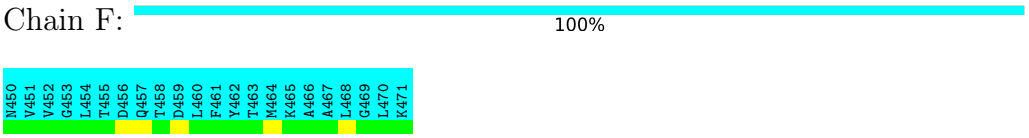


• Molecule 2: Alkaline phosphatase

Chain E:

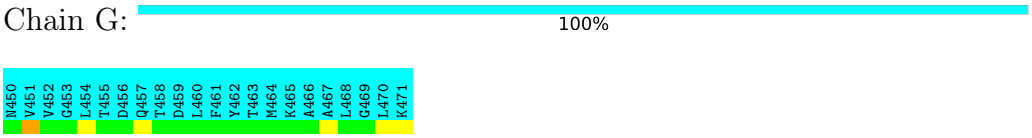
• Molecule 2: Alkaline phosphatase

Chain F:



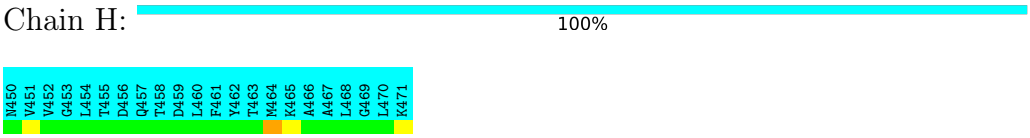
• Molecule 2: Alkaline phosphatase

Chain G:



• Molecule 2: Alkaline phosphatase

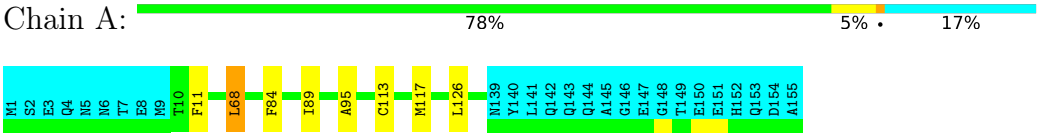
Chain H:



4.2.18 Score per residue for model 18

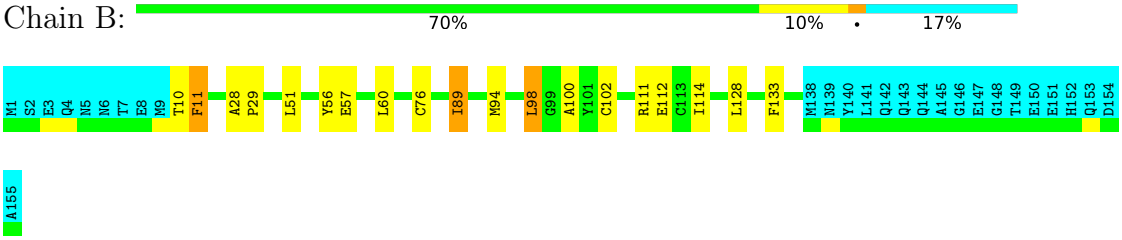
• Molecule 1: Protein-export protein SecB

Chain A:



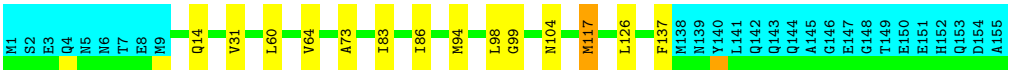
• Molecule 1: Protein-export protein SecB

Chain B:



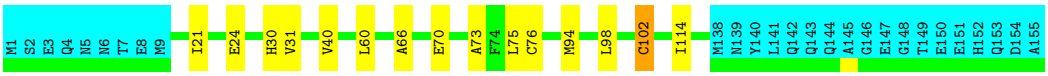
• Molecule 1: Protein-export protein SecB

Chain C:



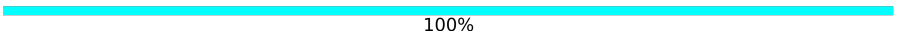
• Molecule 1: Protein-export protein SecB

Chain D:



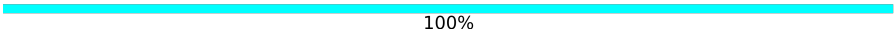
• Molecule 2: Alkaline phosphatase

Chain E:



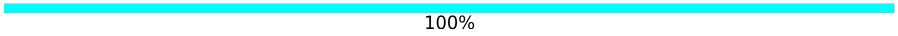
• Molecule 2: Alkaline phosphatase

Chain F:



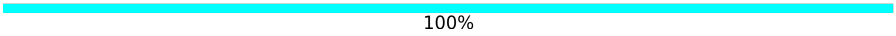
• Molecule 2: Alkaline phosphatase

Chain G:



• Molecule 2: Alkaline phosphatase

Chain H:



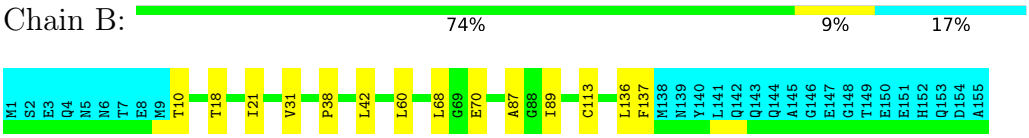
4.2.19 Score per residue for model 19

• Molecule 1: Protein-export protein SecB

Chain A:

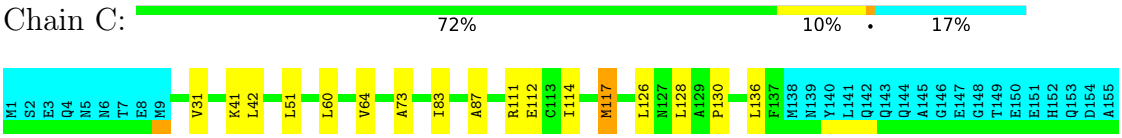
• Molecule 1: Protein-export protein SecB

Chain B:



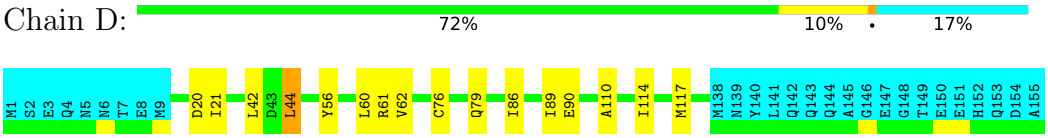
• Molecule 1: Protein-export protein SecB

Chain C:



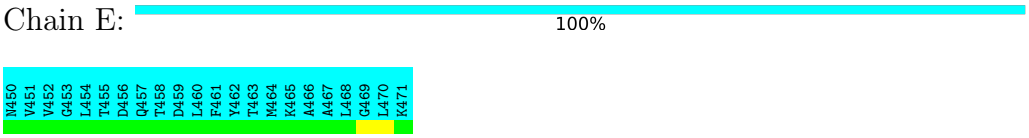
• Molecule 1: Protein-export protein SecB

Chain D:



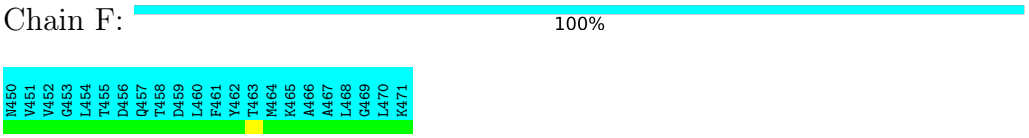
• Molecule 2: Alkaline phosphatase

Chain E:



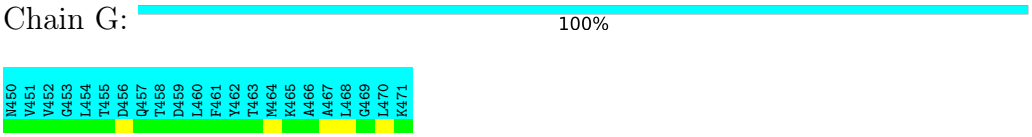
• Molecule 2: Alkaline phosphatase

Chain F:



• Molecule 2: Alkaline phosphatase

Chain G:



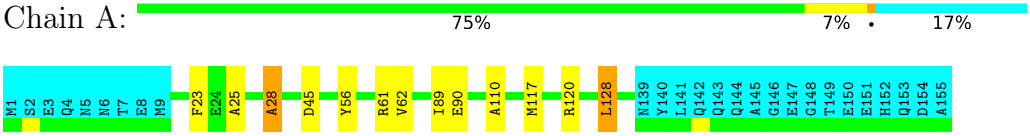
• Molecule 2: Alkaline phosphatase

Chain H:

4.2.20 Score per residue for model 20

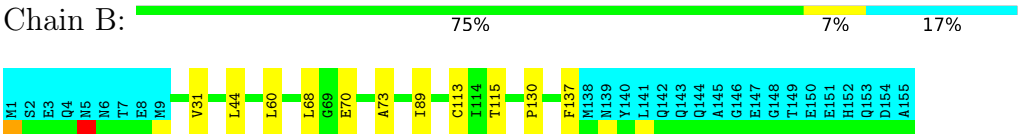
• Molecule 1: Protein-export protein SecB

Chain A:



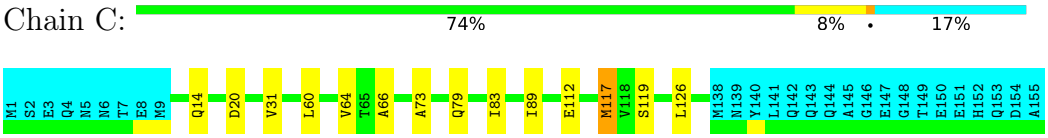
• Molecule 1: Protein-export protein SecB

Chain B:



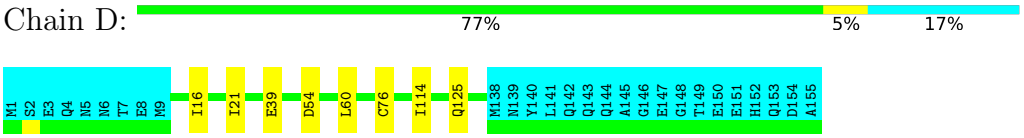
• Molecule 1: Protein-export protein SecB

Chain C:



• Molecule 1: Protein-export protein SecB

Chain D:



• Molecule 2: Alkaline phosphatase

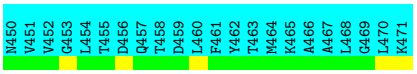
Chain E:

• Molecule 2: Alkaline phosphatase

Chain F:

• Molecule 2: Alkaline phosphatase

Chain G:



• Molecule 2: Alkaline phosphatase

Chain H:

N450
V451
V452
G453
L454
T455
D456
Q457
T458
D459
L460
F461
Y462
T463
M464
K465
A466
A467
L468
G469
L470
K471

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	5048
Number of shifts mapped to atoms	5048
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	14%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.18±0.03	0±1/1029 (0.0± 0.1%)	0.91±0.01	0±0/1403 (0.0± 0.0%)
1	B	1.16±0.02	0±1/1021 (0.0± 0.1%)	0.93±0.02	0±0/1393 (0.0± 0.0%)
1	C	1.16±0.03	0±1/1021 (0.0± 0.1%)	0.94±0.02	0±0/1393 (0.0± 0.0%)
1	D	1.16±0.03	0±0/1021 (0.0± 0.0%)	0.92±0.01	0±0/1393 (0.0± 0.0%)
All	All	1.17	25/81840 (0.0%)	0.92	9/111640 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.2
All	All	0	1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	28	ALA	C-N	7.64	1.40	1.33	20	6
1	C	40	VAL	CA-CB	5.78	1.59	1.53	8	3
1	C	37	GLN	C-N	5.65	1.38	1.33	8	1
1	D	16	ILE	CA-CB	5.34	1.61	1.54	1	1
1	C	86	ILE	CA-CB	5.33	1.61	1.54	15	1
1	B	89	ILE	CA-CB	5.32	1.59	1.54	15	1
1	A	40	VAL	CA-CB	5.30	1.59	1.53	7	1
1	A	129	ALA	C-N	5.22	1.39	1.33	11	1
1	B	86	ILE	CA-CB	5.20	1.61	1.54	15	1
1	B	28	ALA	C-N	5.16	1.40	1.34	13	1
1	D	102	CYS	C-N	5.07	1.40	1.33	8	3
1	B	102	CYS	C-N	5.06	1.40	1.33	6	3
1	A	102	CYS	C-N	5.06	1.40	1.33	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	86	ILE	CA-CB	5.05	1.60	1.54	16	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	11	PHE	CA-CB-CG	8.11	121.91	113.80	1	7
1	D	30	HIS	CA-CB-CG	5.88	119.68	113.80	6	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	10	THR	Peptide	1

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	1005	980	978	5±2
1	B	997	971	969	5±2
1	C	997	971	969	6±2
1	D	997	971	969	5±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	79920	77860	77700	379

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:31:VAL:HG21	1:C:73:ALA:HA	0.68	1.65	6	20
1:C:117:MET:HE3	1:D:21:ILE:HD13	0.65	1.68	19	16
1:B:43:ASP:HB2	1:B:63:THR:HB	0.64	1.68	8	4
1:C:86:ILE:HG21	1:C:97:CYS:SG	0.64	2.32	11	1
1:B:31:VAL:HG21	1:B:73:ALA:HA	0.63	1.70	4	7
1:B:94:MET:HE2	1:B:98:LEU:HD11	0.63	1.71	2	1
1:B:25:ALA:HB1	1:B:28:ALA:HB2	0.61	1.71	15	6
1:B:130:PRO:HG2	1:D:16:ILE:HD13	0.61	1.73	20	2
1:C:34:LYS:HG2	1:C:68:LEU:HD13	0.60	1.73	5	8
1:D:25:ALA:HB1	1:D:28:ALA:HB2	0.58	1.75	4	1
1:C:86:ILE:HD11	1:C:94:MET:HB2	0.57	1.76	9	1
1:A:25:ALA:HB1	1:A:28:ALA:HB2	0.56	1.76	12	3
1:D:76:CYS:SG	1:D:114:ILE:HG12	0.56	2.39	20	10
1:B:25:ALA:CB	1:B:28:ALA:HB2	0.56	2.30	3	5
1:C:64:VAL:HG11	1:C:126:LEU:HD21	0.56	1.78	3	3
1:D:31:VAL:HG21	1:D:73:ALA:HA	0.55	1.76	2	7
1:C:111:ARG:HG2	1:C:128:LEU:HG	0.55	1.77	17	1
1:D:76:CYS:SG	1:D:117:MET:HE3	0.54	2.43	13	3
1:A:86:ILE:HD13	1:A:89:ILE:HD11	0.54	1.79	5	1
1:A:89:ILE:HG13	1:A:97:CYS:SG	0.54	2.43	17	4
1:D:38:PRO:HB2	1:D:66:ALA:HB1	0.53	1.80	2	1
1:B:86:ILE:HD13	1:B:98:LEU:HD11	0.53	1.80	4	1
1:C:64:VAL:HG11	1:C:126:LEU:HD11	0.53	1.80	18	4
1:A:34:LYS:HZ2	1:A:71:GLU:HG3	0.53	1.62	6	1
1:D:64:VAL:HB	1:D:76:CYS:HB2	0.53	1.80	11	1
1:B:18:THR:HG21	1:B:21:ILE:HD11	0.53	1.81	16	4
1:A:61:ARG:HG3	1:A:79:GLN:HG3	0.53	1.80	16	1
1:B:111:ARG:HG3	1:B:128:LEU:HB3	0.53	1.79	10	3
1:A:128:LEU:H	1:A:128:LEU:HD23	0.52	1.63	20	4
1:B:119:SER:HB2	1:C:125:GLN:HE21	0.52	1.65	6	1
1:C:86:ILE:HG12	1:C:98:LEU:HD21	0.52	1.82	16	1
1:A:76:CYS:SG	1:A:118:VAL:HG22	0.52	2.45	9	1
1:D:94:MET:HE1	1:D:98:LEU:HD22	0.52	1.80	3	1
1:B:64:VAL:HG21	1:B:114:ILE:HG21	0.51	1.81	5	3
1:A:45:ASP:HB3	1:A:61:ARG:HB2	0.51	1.82	20	2
1:C:10:THR:HB	1:C:87:ALA:HB3	0.51	1.82	7	2
1:A:68:LEU:H	1:A:68:LEU:HD23	0.51	1.65	18	3
1:A:62:VAL:HG21	1:A:110:ALA:HB1	0.51	1.81	14	2
1:A:120:ARG:HD3	1:B:113:CYS:SG	0.51	2.46	1	3
1:D:100:ALA:HB1	1:D:134:ASP:HA	0.51	1.82	14	4
1:A:64:VAL:HB	1:A:76:CYS:HB2	0.50	1.83	2	1
1:B:31:VAL:HG22	1:B:68:LEU:HD12	0.50	1.83	16	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:118:VAL:HG11	1:C:126:LEU:HD23	0.50	1.83	12	1
1:A:20:ASP:HB3	1:A:79:GLN:HB2	0.50	1.81	19	3
1:D:43:ASP:HB2	1:D:63:THR:HB	0.50	1.83	4	3
1:A:34:LYS:NZ	1:A:71:GLU:HG3	0.50	2.21	6	1
1:C:76:CYS:SG	1:C:114:ILE:HG23	0.49	2.47	9	1
1:D:20:ASP:HB3	1:D:79:GLN:HB2	0.49	1.83	13	3
1:D:94:MET:SD	1:D:95:ALA:N	0.49	2.86	4	1
1:A:45:ASP:HB2	1:A:61:ARG:HB3	0.49	1.84	17	3
1:D:24:GLU:HB2	1:D:75:LEU:HB2	0.49	1.84	6	3
1:A:10:THR:HB	1:A:87:ALA:HB3	0.49	1.84	14	1
1:C:51:LEU:HD11	1:C:83:ILE:HD12	0.49	1.85	19	15
1:D:98:LEU:HA	1:D:102:CYS:SG	0.49	2.47	8	3
1:A:28:ALA:HB3	1:A:29:PRO:HD3	0.48	1.86	17	2
1:D:11:PHE:HE2	1:D:102:CYS:HG	0.48	1.50	11	1
1:A:113:CYS:SG	1:B:120:ARG:HD3	0.48	2.48	9	3
1:B:21:ILE:HD11	1:B:113:CYS:SG	0.48	2.48	3	5
1:C:42:LEU:HD11	1:C:128:LEU:HD12	0.48	1.86	19	1
1:A:23:PHE:HB2	1:A:117:MET:SD	0.48	2.48	20	5
1:A:16:ILE:HD12	1:C:130:PRO:HG3	0.47	1.86	8	2
1:D:76:CYS:SG	1:D:114:ILE:HG23	0.47	2.48	4	5
1:B:51:LEU:HD11	1:B:57:GLU:HB2	0.47	1.86	18	1
1:A:31:VAL:HG21	1:A:73:ALA:HA	0.47	1.86	1	1
1:D:45:ASP:HB3	1:D:61:ARG:HB3	0.46	1.87	11	1
1:A:111:ARG:NH1	1:C:105:ILE:HD12	0.46	2.25	9	4
1:C:11:PHE:HE1	1:C:102:CYS:SG	0.46	2.34	16	2
1:A:31:VAL:HA	1:A:34:LYS:HG2	0.46	1.87	2	1
1:A:11:PHE:HE2	1:A:84:PHE:HB3	0.46	1.70	16	8
1:C:14:GLN:HB2	1:C:83:ILE:HB	0.46	1.88	9	5
1:B:86:ILE:HB	1:B:89:ILE:HD11	0.46	1.88	11	3
1:A:20:ASP:HB2	1:A:79:GLN:HB2	0.46	1.86	5	1
1:B:28:ALA:HB3	1:B:29:PRO:HD3	0.45	1.88	6	6
1:A:31:VAL:HG23	1:A:68:LEU:HD12	0.45	1.88	11	1
1:A:23:PHE:HA	1:A:75:LEU:O	0.45	2.11	7	1
1:D:98:LEU:HD13	1:D:102:CYS:SG	0.45	2.52	18	1
1:C:111:ARG:HG3	1:C:128:LEU:HB2	0.45	1.87	19	1
1:C:76:CYS:SG	1:C:114:ILE:HA	0.45	2.52	13	1
1:A:100:ALA:HB1	1:A:134:ASP:HA	0.45	1.89	16	1
1:C:19:LYS:HD3	1:C:81:GLY:HA3	0.44	1.89	1	2
1:B:40:VAL:HG13	1:B:64:VAL:HG13	0.44	1.89	2	1
1:C:117:MET:HE2	1:D:21:ILE:HG21	0.44	1.89	2	1
1:D:44:LEU:H	1:D:44:LEU:HD13	0.44	1.71	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:21:ILE:HG21	1:C:117:MET:HE2	0.44	1.88	12	1
1:A:90:GLU:HA	1:A:94:MET:HE3	0.44	1.87	2	1
1:D:23:PHE:HB2	1:D:117:MET:SD	0.44	2.52	6	3
1:B:76:CYS:SG	1:B:114:ILE:HG23	0.44	2.53	18	2
1:A:31:VAL:HG11	1:A:73:ALA:HA	0.44	1.88	15	1
1:C:98:LEU:HA	1:C:102:CYS:SG	0.44	2.53	16	1
1:D:40:VAL:HG13	1:D:64:VAL:HG13	0.44	1.87	10	1
1:A:44:LEU:HD22	1:A:62:VAL:HG12	0.44	1.89	19	1
1:D:47:ALA:HB3	1:D:59:VAL:HB	0.43	1.90	3	2
1:B:94:MET:C	1:B:94:MET:SD	0.43	3.01	18	1
1:D:31:VAL:HG22	1:D:68:LEU:HD12	0.43	1.91	2	2
1:B:42:LEU:H	1:B:42:LEU:HD23	0.43	1.74	11	1
1:A:43:ASP:HB3	1:A:63:THR:HB	0.43	1.90	16	1
1:B:89:ILE:HD13	1:B:89:ILE:H	0.43	1.73	18	1
1:D:61:ARG:HG2	1:D:79:GLN:HG2	0.43	1.90	19	1
1:B:38:PRO:HB3	1:B:68:LEU:HG	0.43	1.91	5	5
1:C:89:ILE:H	1:C:89:ILE:HD13	0.43	1.73	5	2
1:A:79:GLN:HE21	1:A:79:GLN:N	0.43	2.11	6	1
1:B:62:VAL:HB	1:B:114:ILE:HD11	0.43	1.89	5	1
1:D:21:ILE:CG2	1:D:117:MET:SD	0.43	3.07	19	3
1:B:10:THR:HB	1:B:87:ALA:HB3	0.43	1.88	19	2
1:B:113:CYS:O	1:B:117:MET:HG2	0.43	2.14	4	2
1:B:111:ARG:HG3	1:B:128:LEU:HB2	0.43	1.90	18	1
1:D:62:VAL:HG21	1:D:110:ALA:HB1	0.43	1.90	19	1
1:C:36:TRP:NE1	1:C:124:PRO:HG3	0.42	2.28	2	1
1:A:44:LEU:HD23	1:A:62:VAL:HG22	0.42	1.90	6	1
1:B:98:LEU:HD12	1:B:99:GLY:N	0.42	2.29	10	1
1:D:42:LEU:HD23	1:D:42:LEU:H	0.42	1.73	19	1
1:A:13:ILE:CD1	1:A:105:ILE:HG21	0.42	2.44	14	1
1:B:115:THR:HG21	1:C:119:SER:OG	0.42	2.14	15	2
1:C:30:HIS:O	1:C:33:GLN:HG2	0.42	2.13	7	1
1:B:125:GLN:HB2	1:C:124:PRO:HA	0.42	1.92	6	1
1:B:94:MET:O	1:B:98:LEU:HG	0.42	2.14	7	1
1:A:97:CYS:HA	1:A:101:TYR:HB3	0.42	1.91	9	2
1:A:64:VAL:O	1:A:75:LEU:HD12	0.42	2.15	12	1
1:A:43:ASP:HB2	1:A:63:THR:HB	0.42	1.91	1	1
1:C:62:VAL:HB	1:C:114:ILE:HD11	0.42	1.91	2	2
1:A:61:ARG:HG3	1:A:79:GLN:HG2	0.42	1.91	17	1
1:C:64:VAL:HG21	1:C:114:ILE:HG21	0.42	1.91	19	1
1:B:89:ILE:H	1:B:89:ILE:HD13	0.42	1.75	1	1
1:D:28:ALA:O	1:D:31:VAL:HG12	0.42	2.15	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:34:LYS:NZ	1:C:71:GLU:HG2	0.42	2.30	15	1
1:C:90:GLU:HA	1:C:94:MET:HB2	0.42	1.91	16	1
1:A:13:ILE:HD11	1:A:105:ILE:HG21	0.41	1.92	2	1
1:B:24:GLU:HB2	1:B:75:LEU:HB2	0.41	1.90	10	2
1:B:41:LYS:HB3	1:B:65:THR:HB	0.41	1.92	5	1
1:B:21:ILE:CD1	1:B:113:CYS:SG	0.41	3.08	12	1
1:B:100:ALA:HB1	1:B:134:ASP:HA	0.41	1.93	12	1
1:C:17:TYR:CE2	1:C:19:LYS:HD3	0.41	2.50	15	2
1:A:96:HIS:NE2	1:A:100:ALA:HB3	0.41	2.29	17	1
1:C:20:ASP:HB3	1:C:79:GLN:HB2	0.41	1.91	20	1
1:A:64:VAL:HG21	1:A:114:ILE:HG21	0.41	1.91	1	1
1:D:48:SER:HB3	1:D:98:LEU:HD21	0.41	1.92	17	1
1:A:96:HIS:O	1:A:100:ALA:HB3	0.41	2.16	5	1
1:A:21:ILE:HB	1:B:23:PHE:HB3	0.41	1.92	11	1
1:D:11:PHE:HE2	1:D:102:CYS:SG	0.41	2.38	11	1
1:A:23:PHE:HB3	1:B:21:ILE:HB	0.41	1.91	3	1
1:C:118:VAL:HG21	1:C:126:LEU:HD12	0.41	1.92	15	1
1:A:86:ILE:HD13	1:A:94:MET:SD	0.41	2.56	3	1
1:A:90:GLU:HA	1:A:94:MET:SD	0.41	2.55	11	1
1:C:56:TYR:HB2	1:C:86:ILE:HD11	0.41	1.92	15	1
1:C:86:ILE:HD13	1:C:98:LEU:HD11	0.41	1.93	18	1
1:A:117:MET:HA	1:A:117:MET:HE2	0.41	1.92	20	1
1:D:40:VAL:HG23	1:D:64:VAL:HG13	0.41	1.91	4	2
1:C:31:VAL:O	1:C:34:LYS:HB2	0.41	2.16	7	1
1:B:80:GLN:HG2	1:B:109:TYR:HB2	0.41	1.92	15	1
1:C:45:ASP:HB3	1:C:61:ARG:HB3	0.41	1.93	1	1
1:C:100:ALA:HB1	1:C:134:ASP:HA	0.41	1.92	5	1
1:C:11:PHE:HE1	1:C:102:CYS:HG	0.41	1.54	7	1
1:A:51:LEU:HD11	1:A:57:GLU:HB2	0.41	1.91	11	1
1:C:86:ILE:H	1:C:86:ILE:HD13	0.41	1.76	13	1
1:C:25:ALA:HB1	1:C:28:ALA:HB2	0.41	1.92	15	1
1:A:113:CYS:O	1:A:117:MET:HG2	0.41	2.16	18	1
1:D:13:ILE:HD11	1:D:105:ILE:HD13	0.41	1.92	3	1
1:B:119:SER:HB2	1:C:125:GLN:NE2	0.41	2.31	6	1
1:B:97:CYS:SG	1:B:102:CYS:SG	0.41	3.18	8	1
1:A:34:LYS:HZ3	1:A:68:LEU:HD12	0.41	1.76	9	1
1:C:43:ASP:HB3	1:C:63:THR:HB	0.41	1.92	16	1
1:C:51:LEU:HD11	1:C:57:GLU:HB2	0.41	1.93	16	1
1:D:16:ILE:N	1:D:16:ILE:HD12	0.40	2.31	6	1
1:C:64:VAL:HG23	1:C:114:ILE:HD13	0.40	1.92	13	1
1:B:89:ILE:HD12	1:B:94:MET:HA	0.40	1.93	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:100:ALA:HA	1:B:133:PHE:HB3	0.40	1.93	18	1
1:C:66:ALA:HB3	1:C:73:ALA:HB3	0.40	1.93	20	1
1:B:38:PRO:HB2	1:B:66:ALA:HB1	0.40	1.92	4	1
1:A:61:ARG:HB2	1:A:79:GLN:HG2	0.40	1.93	15	1
1:A:28:ALA:HB1	1:B:17:TYR:CE2	0.40	2.51	16	1
1:B:105:ILE:HG23	1:D:111:ARG:NH2	0.40	2.31	1	1
1:B:86:ILE:HD13	1:B:98:LEU:HD21	0.40	1.92	12	1
1:D:40:VAL:HG12	1:D:66:ALA:HB2	0.40	1.92	18	1
1:C:11:PHE:HE2	1:C:84:PHE:HB3	0.40	1.76	2	1
1:A:31:VAL:HG22	1:A:68:LEU:HD21	0.40	1.92	13	1
1:C:104:ASN:ND2	1:C:134:ASP:HB2	0.40	2.31	13	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	129/155 (83%)	124±2 (96±1%)	5±2 (4±1%)	0±0 (0±0%)	100	100
1	B	128/155 (83%)	120±2 (94±1%)	7±2 (6±1%)	0±0 (0±0%)	49	83
1	C	128/155 (83%)	121±3 (94±2%)	7±2 (6±2%)	0±1 (0±0%)	44	80
1	D	128/155 (83%)	122±1 (95±1%)	6±1 (4±1%)	0±0 (0±0%)	37	78
2	E	0	-	-	-	-	
2	F	0	-	-	-	-	
2	G	0	-	-	-	-	
2	H	0	-	-	-	-	
All	All	10260/14160 (72%)	9741 (95%)	503 (5%)	16 (0%)	44	80

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	28	ALA	7
1	C	130	PRO	3
1	B	28	ALA	2

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Mol	Chain	Res	Type	Models (Total)
1	C	100	ALA	1
1	B	124	PRO	1
1	D	91	GLY	1
1	A	130	PRO	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	110/132 (83%)	107±1 (98±1%)	3±1 (2±1%)	42 88
1	B	109/132 (83%)	106±2 (97±2%)	3±2 (3±2%)	38 86
1	C	109/132 (83%)	105±1 (96±1%)	4±1 (4±1%)	29 79
1	D	109/132 (83%)	106±1 (97±1%)	3±1 (3±1%)	40 87
2	E	0	-	-	-
2	F	0	-	-	-
2	G	0	-	-	-
2	H	0	-	-	-
All	All	8740/12000 (73%)	8476 (97%)	264 (3%)	37 85

All 72 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	B	60	LEU	20
1	C	60	LEU	20
1	D	60	LEU	20
1	A	89	ILE	18
1	C	117	MET	18
1	D	70	GLU	9
1	C	34	LYS	8
1	D	90	GLU	8
1	A	68	LEU	8
1	C	89	ILE	7
1	D	89	ILE	7
1	C	112	GLU	7
1	B	44	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	B	89	ILE	6
1	A	90	GLU	6
1	B	112	GLU	6
1	C	86	ILE	5
1	B	11	PHE	4
1	C	128	LEU	4
1	B	12	GLN	3
1	A	138	MET	3
1	D	86	ILE	3
1	C	136	LEU	3
1	A	128	LEU	3
1	A	56	TYR	3
1	C	19	LYS	2
1	A	34	LYS	2
1	B	86	ILE	2
1	B	42	LEU	2
1	A	125	GLN	2
1	D	42	LEU	2
1	C	41	LYS	2
1	A	60	LEU	2
1	C	12	GLN	2
1	B	56	TYR	2
1	D	56	TYR	2
1	B	70	GLU	2
1	A	86	ILE	1
1	B	37	GLN	1
1	B	90	GLU	1
1	B	113	CYS	1
1	B	126	LEU	1
1	C	37	GLN	1
1	A	37	GLN	1
1	D	136	LEU	1
1	C	77	GLU	1
1	D	126	LEU	1
1	A	79	GLN	1
1	B	53	ASP	1
1	D	16	ILE	1
1	D	30	HIS	1
1	C	46	THR	1
1	C	61	ARG	1
1	C	127	ASN	1
1	B	127	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	98	LEU	1
1	C	68	LEU	1
1	D	40	VAL	1
1	C	40	VAL	1
1	D	128	LEU	1
1	C	126	LEU	1
1	A	70	GLU	1
1	C	56	TYR	1
1	A	61	ARG	1
1	B	128	LEU	1
1	B	136	LEU	1
1	B	98	LEU	1
1	C	104	ASN	1
1	A	14	GLN	1
1	A	93	GLN	1
1	D	44	LEU	1
1	D	125	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues (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 14% for the well-defined parts and 14% 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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	139	0.25 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.84 ± 0.22	Should be checked
$^{13}C'$	137	0.29 ± 0.15	None needed (< 0.5 ppm)
^{15}N	133	-1.16 ± 0.25	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 14%, i.e. 932 atoms were assigned a chemical shift out of a possible 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	475/2537 (19%)	116/1026 (11%)	243/1026 (24%)	116/485 (24%)
Sidechain	388/3714 (10%)	216/2435 (9%)	172/1167 (15%)	0/112 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	69/616 (11%)	35/300 (12%)	33/296 (11%)	1/20 (5%)
Overall	932/6867 (14%)	367/3761 (10%)	448/2489 (18%)	117/617 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1046 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	542/3528 (15%)	133/1432 (9%)	276/1416 (19%)	133/680 (20%)
Sidechain	427/5092 (8%)	234/3320 (7%)	193/1612 (12%)	0/160 (0%)
Aromatic	77/760 (10%)	39/368 (11%)	37/364 (10%)	1/28 (4%)
Overall	1046/9380 (11%)	406/5120 (8%)	506/3392 (15%)	134/868 (15%)

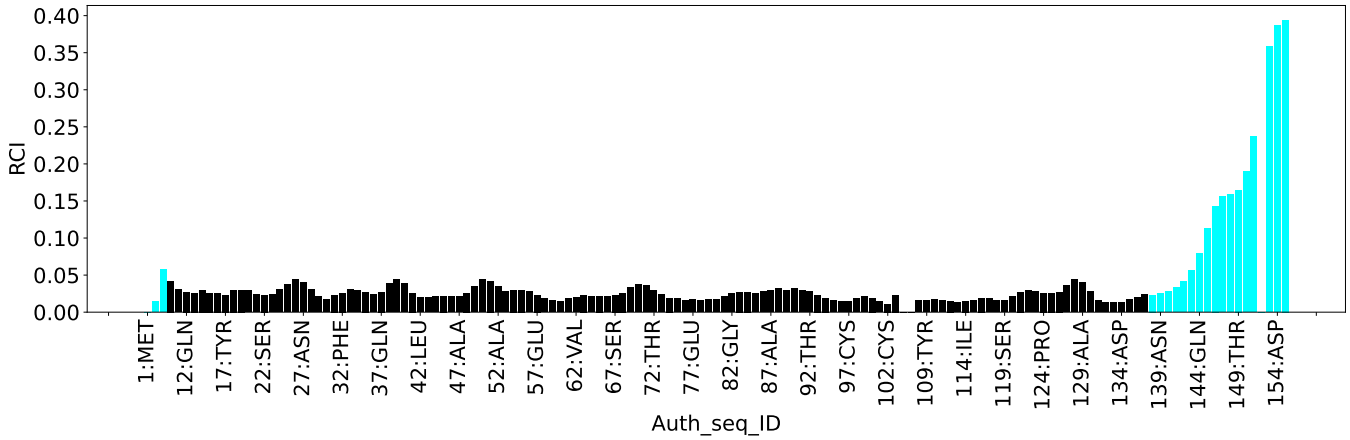
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	140	0.27 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	126	0.78 ± 0.20	Should be checked
$^{13}C'$	135	0.26 ± 0.12	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.27	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. 927 atoms were assigned a chemical shift out of a possible 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	472/2537 (19%)	115/1026 (11%)	242/1026 (24%)	115/485 (24%)
Sidechain	386/3714 (10%)	216/2435 (9%)	170/1167 (15%)	0/112 (0%)
Aromatic	69/616 (11%)	35/300 (12%)	33/296 (11%)	1/20 (5%)
Overall	927/6867 (13%)	366/3761 (10%)	445/2489 (18%)	116/617 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1044 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	539/3528 (15%)	132/1432 (9%)	275/1416 (19%)	132/680 (19%)
Sidechain	428/5092 (8%)	237/3320 (7%)	191/1612 (12%)	0/160 (0%)
Aromatic	77/760 (10%)	39/368 (11%)	37/364 (10%)	1/28 (4%)
Overall	1044/9380 (11%)	408/5120 (8%)	503/3392 (15%)	133/868 (15%)

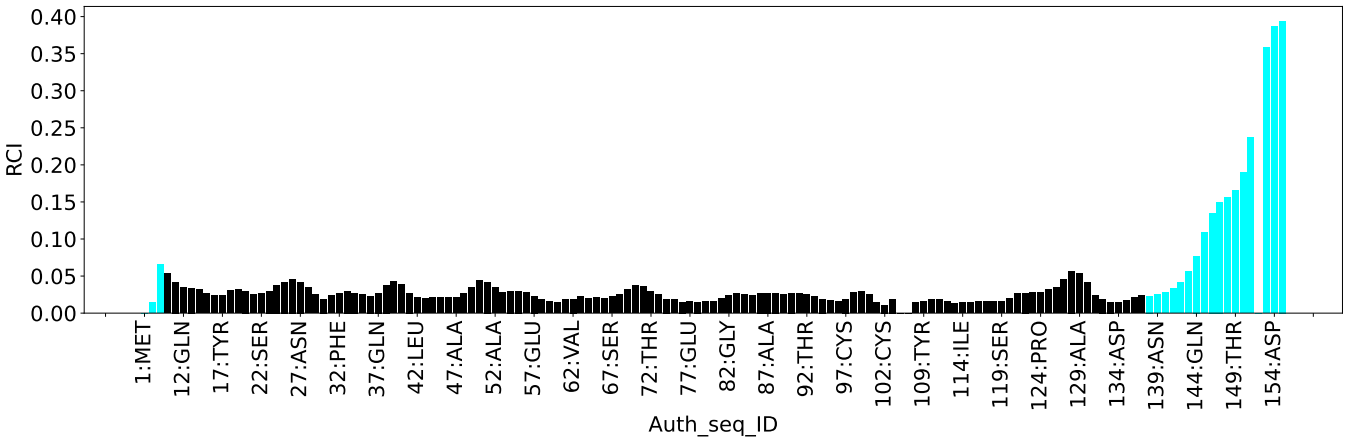
7.2.4 Statistically unusual chemical shifts (i)

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 A:



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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	140	0.27 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	126	0.78 ± 0.20	Should be checked
$^{13}C'$	135	0.26 ± 0.12	None needed (< 0.5 ppm)
^{15}N	132	-1.09 ± 0.27	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. 927 atoms were assigned a chemical shift out of a possible 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	472/2537 (19%)	115/1026 (11%)	242/1026 (24%)	115/485 (24%)
Sidechain	386/3714 (10%)	216/2435 (9%)	170/1167 (15%)	0/112 (0%)
Aromatic	69/616 (11%)	35/300 (12%)	33/296 (11%)	1/20 (5%)
Overall	927/6867 (13%)	366/3761 (10%)	445/2489 (18%)	116/617 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1044 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	539/3528 (15%)	132/1432 (9%)	275/1416 (19%)	132/680 (19%)
Sidechain	428/5092 (8%)	237/3320 (7%)	191/1612 (12%)	0/160 (0%)
Aromatic	77/760 (10%)	39/368 (11%)	37/364 (10%)	1/28 (4%)
Overall	1044/9380 (11%)	408/5120 (8%)	503/3392 (15%)	133/868 (15%)

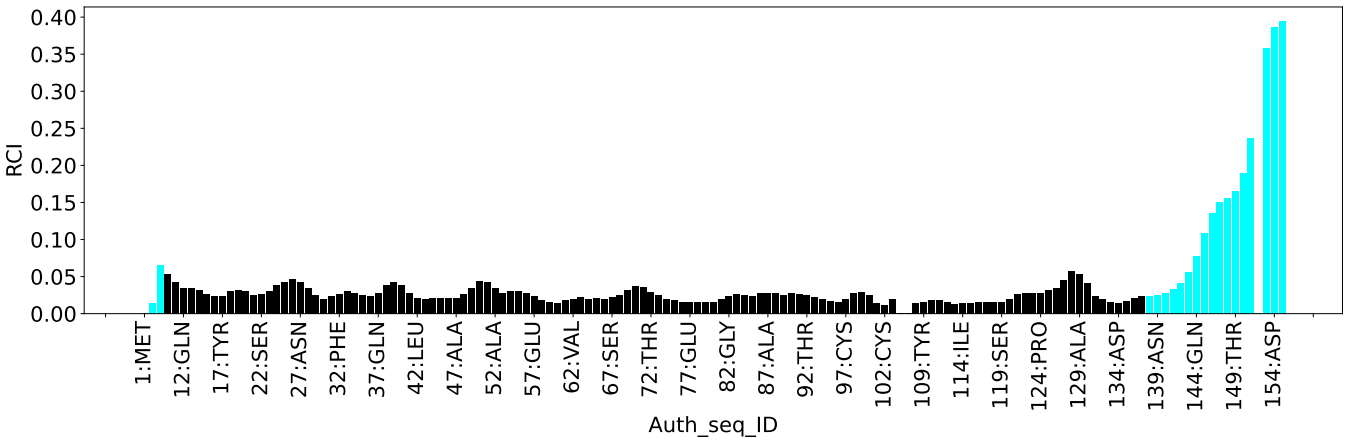
7.3.4 Statistically unusual chemical shifts (i)

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 A:



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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	139	0.25 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	128	0.84 ± 0.22	Should be checked
$^{13}C'$	137	0.29 ± 0.15	None needed (< 0.5 ppm)
^{15}N	133	-1.16 ± 0.25	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 14%, i.e. 932 atoms were assigned a chemical shift out of a possible 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	475/2537 (19%)	116/1026 (11%)	243/1026 (24%)	116/485 (24%)
Sidechain	388/3714 (10%)	216/2435 (9%)	172/1167 (15%)	0/112 (0%)
Aromatic	69/616 (11%)	35/300 (12%)	33/296 (11%)	1/20 (5%)
Overall	932/6867 (14%)	367/3761 (10%)	448/2489 (18%)	117/617 (19%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 1046 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	542/3528 (15%)	133/1432 (9%)	276/1416 (19%)	133/680 (20%)
Sidechain	427/5092 (8%)	234/3320 (7%)	193/1612 (12%)	0/160 (0%)
Aromatic	77/760 (10%)	39/368 (11%)	37/364 (10%)	1/28 (4%)
Overall	1046/9380 (11%)	406/5120 (8%)	506/3392 (15%)	134/868 (15%)

7.4.4 Statistically unusual chemical shifts (i)

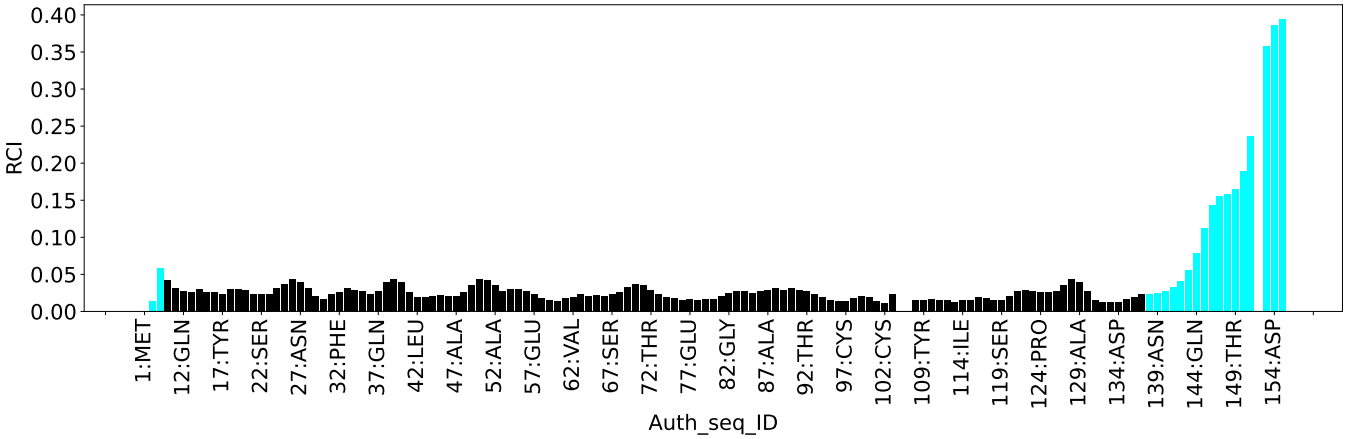
There are no statistically unusual chemical shifts.

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 A:



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	217
Number of shifts mapped to atoms	217
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

No chemical shift referencing corrections were calculated (not enough data).

7.5.3 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 0%, i.e. 0 atoms were assigned a chemical

shift out of a possible 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2537 (0%)	0/1026 (0%)	0/1026 (0%)	0/485 (0%)
Sidechain	0/3714 (0%)	0/2435 (0%)	0/1167 (0%)	0/112 (0%)
Aromatic	0/616 (0%)	0/300 (0%)	0/296 (0%)	0/20 (0%)
Overall	0/6867 (0%)	0/3761 (0%)	0/2489 (0%)	0/617 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 216 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	101/3528 (3%)	40/1432 (3%)	39/1416 (3%)	22/680 (3%)
Sidechain	110/5092 (2%)	66/3320 (2%)	44/1612 (3%)	0/160 (0%)
Aromatic	5/760 (1%)	5/368 (1%)	0/364 (0%)	0/28 (0%)
Overall	216/9380 (2%)	111/5120 (2%)	83/3392 (2%)	22/868 (3%)

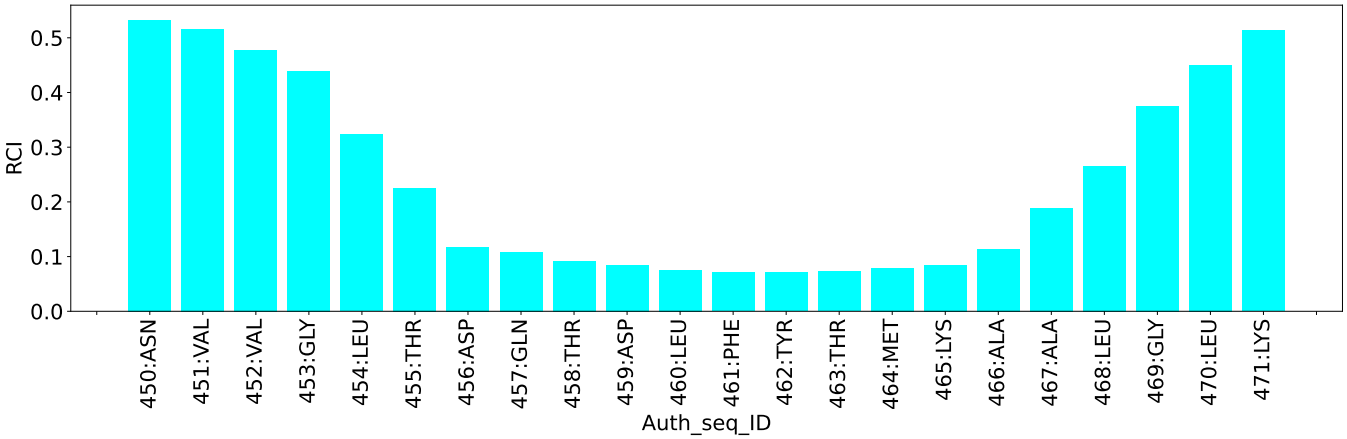
7.5.4 Statistically unusual chemical shifts (i)

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

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	217
Number of shifts mapped to atoms	217
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

No chemical shift referencing corrections were calculated (not enough data).

7.6.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2537 (0%)	0/1026 (0%)	0/1026 (0%)	0/485 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	0/3714 (0%)	0/2435 (0%)	0/1167 (0%)	0/112 (0%)
Aromatic	0/616 (0%)	0/300 (0%)	0/296 (0%)	0/20 (0%)
Overall	0/6867 (0%)	0/3761 (0%)	0/2489 (0%)	0/617 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 216 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	101/3528 (3%)	40/1432 (3%)	39/1416 (3%)	22/680 (3%)
Sidechain	110/5092 (2%)	66/3320 (2%)	44/1612 (3%)	0/160 (0%)
Aromatic	5/760 (1%)	5/368 (1%)	0/364 (0%)	0/28 (0%)
Overall	216/9380 (2%)	111/5120 (2%)	83/3392 (2%)	22/868 (3%)

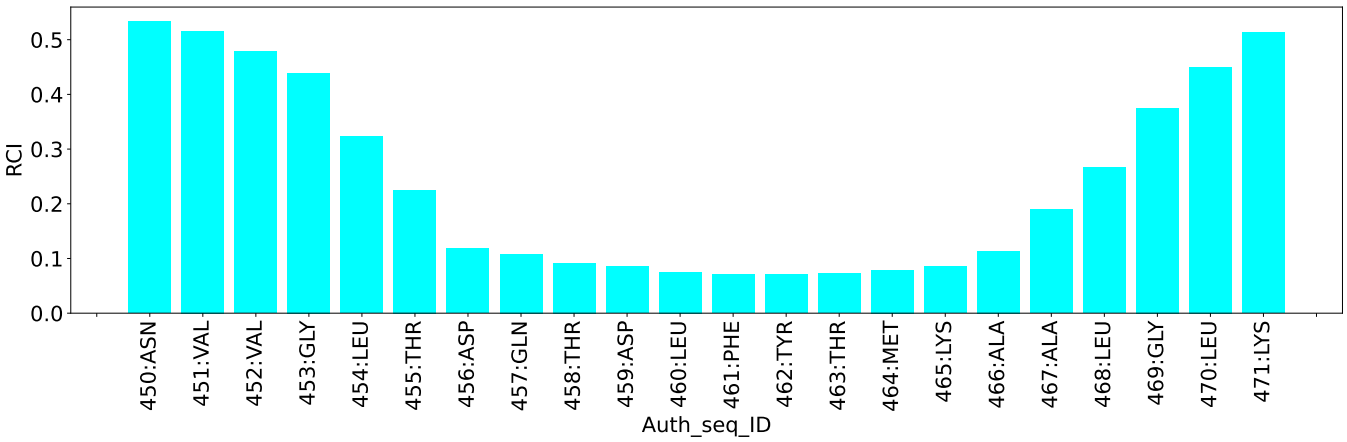
7.6.4 Statistically unusual chemical shifts (i)

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 E:



7.7 Chemical shift list 7

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shift_7*

7.7.1 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	217
Number of shifts mapped to atoms	217
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

No chemical shift referencing corrections were calculated (not enough data).

7.7.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2537 (0%)	0/1026 (0%)	0/1026 (0%)	0/485 (0%)
Sidechain	0/3714 (0%)	0/2435 (0%)	0/1167 (0%)	0/112 (0%)
Aromatic	0/616 (0%)	0/300 (0%)	0/296 (0%)	0/20 (0%)
Overall	0/6867 (0%)	0/3761 (0%)	0/2489 (0%)	0/617 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 216 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	101/3528 (3%)	40/1432 (3%)	39/1416 (3%)	22/680 (3%)
Sidechain	110/5092 (2%)	66/3320 (2%)	44/1612 (3%)	0/160 (0%)
Aromatic	5/760 (1%)	5/368 (1%)	0/364 (0%)	0/28 (0%)
Overall	216/9380 (2%)	111/5120 (2%)	83/3392 (2%)	22/868 (3%)

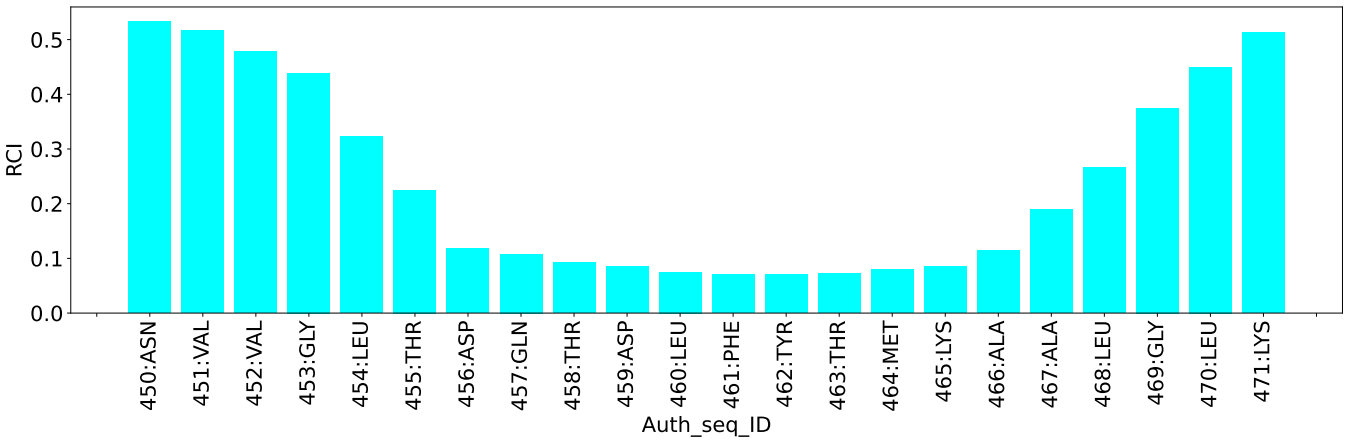
7.7.4 Statistically unusual chemical shifts (i)

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 E:



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	217
Number of shifts mapped to atoms	217
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)

No chemical shift referencing corrections were calculated (not enough data).

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 6867. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/2537 (0%)	0/1026 (0%)	0/1026 (0%)	0/485 (0%)
Sidechain	0/3714 (0%)	0/2435 (0%)	0/1167 (0%)	0/112 (0%)
Aromatic	0/616 (0%)	0/300 (0%)	0/296 (0%)	0/20 (0%)
Overall	0/6867 (0%)	0/3761 (0%)	0/2489 (0%)	0/617 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 216 atoms were assigned a chemical shift out of a possible 9380. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	101/3528 (3%)	40/1432 (3%)	39/1416 (3%)	22/680 (3%)
Sidechain	110/5092 (2%)	66/3320 (2%)	44/1612 (3%)	0/160 (0%)
Aromatic	5/760 (1%)	5/368 (1%)	0/364 (0%)	0/28 (0%)
Overall	216/9380 (2%)	111/5120 (2%)	83/3392 (2%)	22/868 (3%)

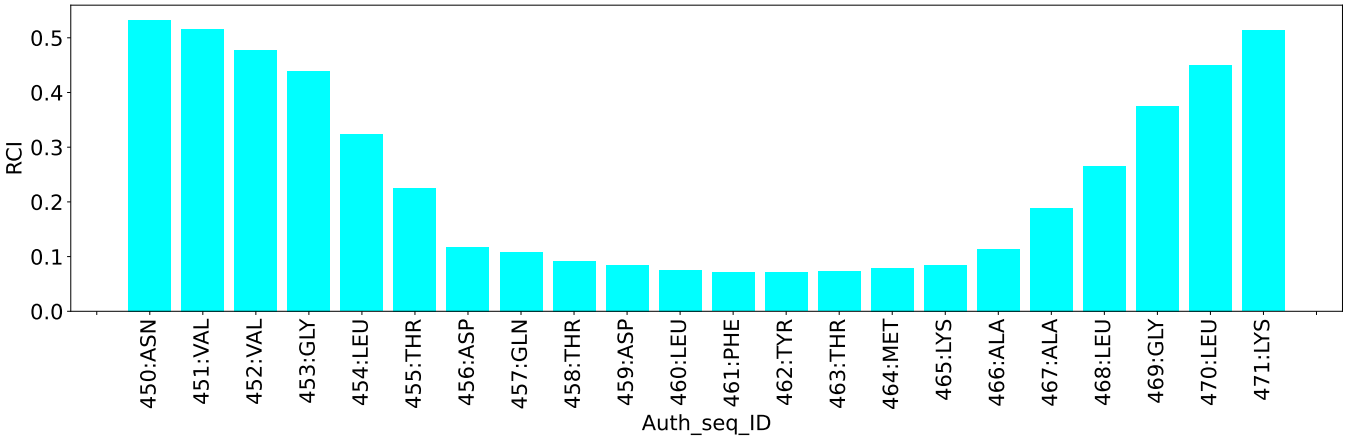
7.8.4 Statistically unusual chemical shifts (i)

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 E:


RCI
0.0
0.1
0.2
0.3
0.4
0.5
450:ASN
451:VAL
452:VAL
453:GLY
454:LEU
455:THR
456:ASP
457:GLN
458:THR
459:ASP
460:LEU
461:PHE
462:TYR
463:THR
464:MET
465:LYS
466:ALA
467:ALA
468:LEU
469:GLY
470:LEU
471:LYS
Auth_seq_ID

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	1689
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	662
Medium range (|i-j|>1 and |i-j|<5)	360
Long range (|i-j|≥5)	520
Inter-chain	147
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	1012
Number of unmapped restraints	0
Number of restraints per residue	3.8
Number of long range restraints per residue[1]	0.7

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	57.5	0.2
0.2-0.5 (Medium)	76.2	0.5
>0.5 (Large)	62.1	9.03

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)	91.3	9.43
10.0-20.0 (Medium)	0.1	12.15
>20.0 (Large)	None	None

9 Distance violation analysis (i)

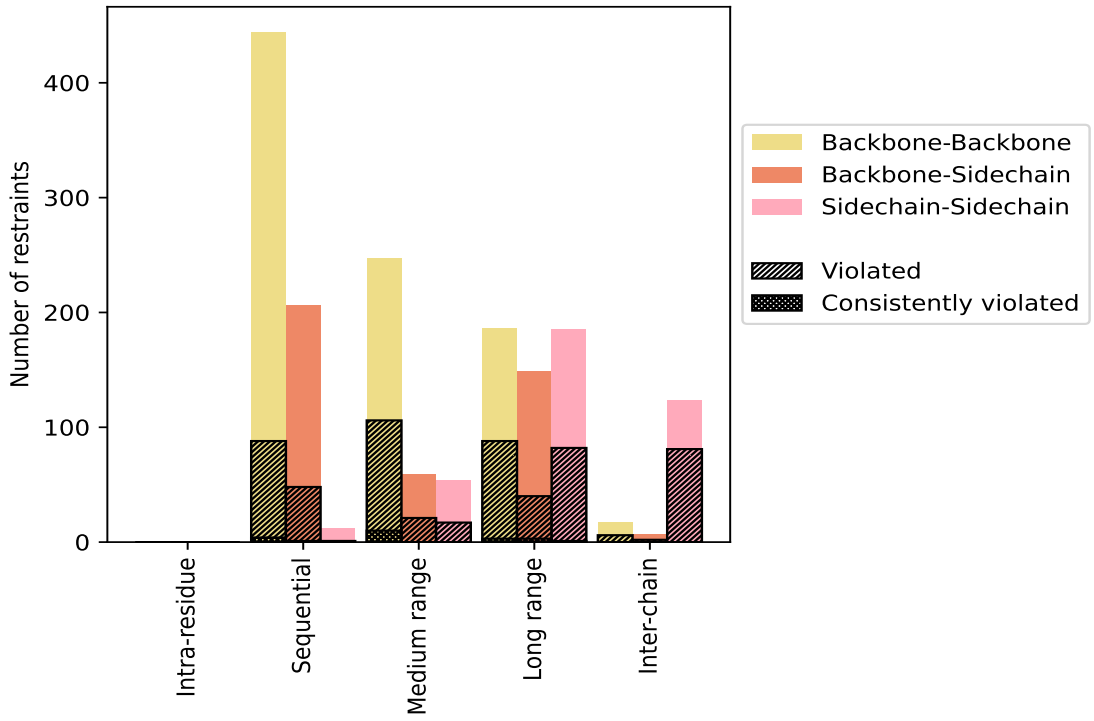
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	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
Sequential (|i-j|=1)	662	39.2	137	20.7	8.1	5	0.8	0.3
Backbone-Backbone	444	26.3	88	19.8	5.2	4	0.9	0.2
Backbone-Sidechain	206	12.2	48	23.3	2.8	1	0.5	0.1
Sidechain-Sidechain	12	0.7	1	8.3	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	360	21.3	144	40.0	8.5	10	2.8	0.6
Backbone-Backbone	247	14.6	106	42.9	6.3	10	4.0	0.6
Backbone-Sidechain	59	3.5	21	35.6	1.2	0	0.0	0.0
Sidechain-Sidechain	54	3.2	17	31.5	1.0	0	0.0	0.0
Long range (|i-j|≥5)	520	30.8	210	40.4	12.4	7	1.3	0.4
Backbone-Backbone	186	11.0	88	47.3	5.2	3	1.6	0.2
Backbone-Sidechain	149	8.8	40	26.8	2.4	3	2.0	0.2
Sidechain-Sidechain	185	11.0	82	44.3	4.9	1	0.5	0.1
Inter-chain	147	8.7	89	60.5	5.3	0	0.0	0.0
Backbone-Backbone	17	1.0	6	35.3	0.4	0	0.0	0.0
Backbone-Sidechain	7	0.4	2	28.6	0.1	0	0.0	0.0
Sidechain-Sidechain	123	7.3	81	65.9	4.8	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1689	100.0	580	34.3	34.3	22	1.3	1.3
Backbone-Backbone	894	52.9	288	32.2	17.1	17	1.9	1.0
Backbone-Sidechain	421	24.9	111	26.4	6.6	4	1.0	0.2
Sidechain-Sidechain	374	22.1	181	48.4	10.7	1	0.3	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	59	46	67	17	189	0.57	4.17	0.7	0.3
2	0	56	50	70	21	197	0.58	4.31	0.68	0.3
3	0	56	57	72	16	201	0.54	3.69	0.59	0.31
4	0	53	54	66	9	182	0.55	4.58	0.66	0.3
5	0	47	50	72	12	181	0.59	4.22	0.67	0.33
6	0	51	50	74	16	191	0.56	4.45	0.61	0.31
7	0	55	59	90	18	222	0.6	4.13	0.7	0.32
8	0	51	56	70	15	192	0.5	3.54	0.54	0.3
9	0	54	51	73	16	194	0.64	3.82	0.74	0.32
10	0	53	68	79	17	217	0.57	4.66	0.68	0.3

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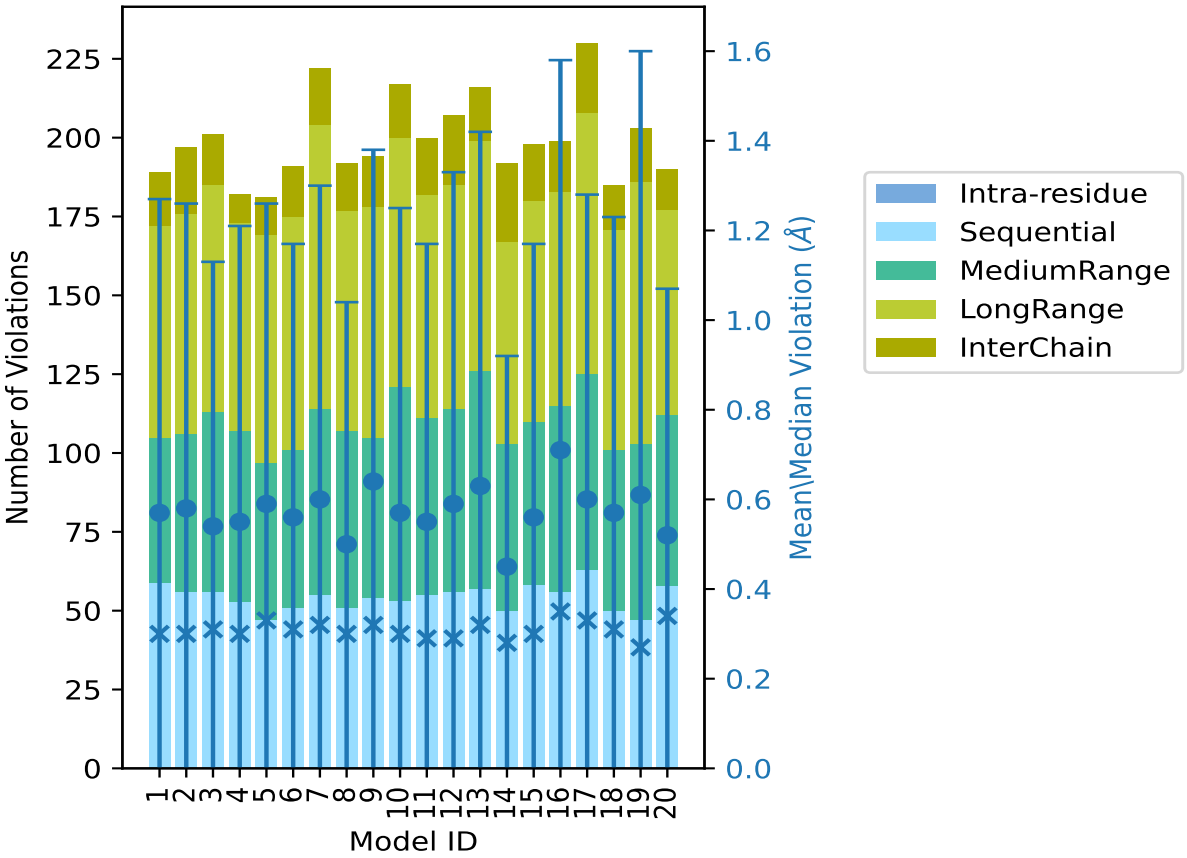
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	55	56	71	18	200	0.55	4.0	0.62	0.29
12	0	56	58	71	22	207	0.59	4.41	0.74	0.29
13	0	57	69	73	17	216	0.63	4.76	0.79	0.32
14	0	50	53	64	25	192	0.45	2.7	0.47	0.28
15	0	58	52	70	18	198	0.56	2.89	0.61	0.3
16	0	56	59	68	16	199	0.71	4.77	0.87	0.35
17	0	63	62	83	22	230	0.6	3.81	0.68	0.33
18	0	50	51	70	14	185	0.57	4.82	0.66	0.31
19	0	47	56	83	17	203	0.61	9.03	0.99	0.27
20	0	58	54	65	13	190	0.52	3.46	0.55	0.34

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

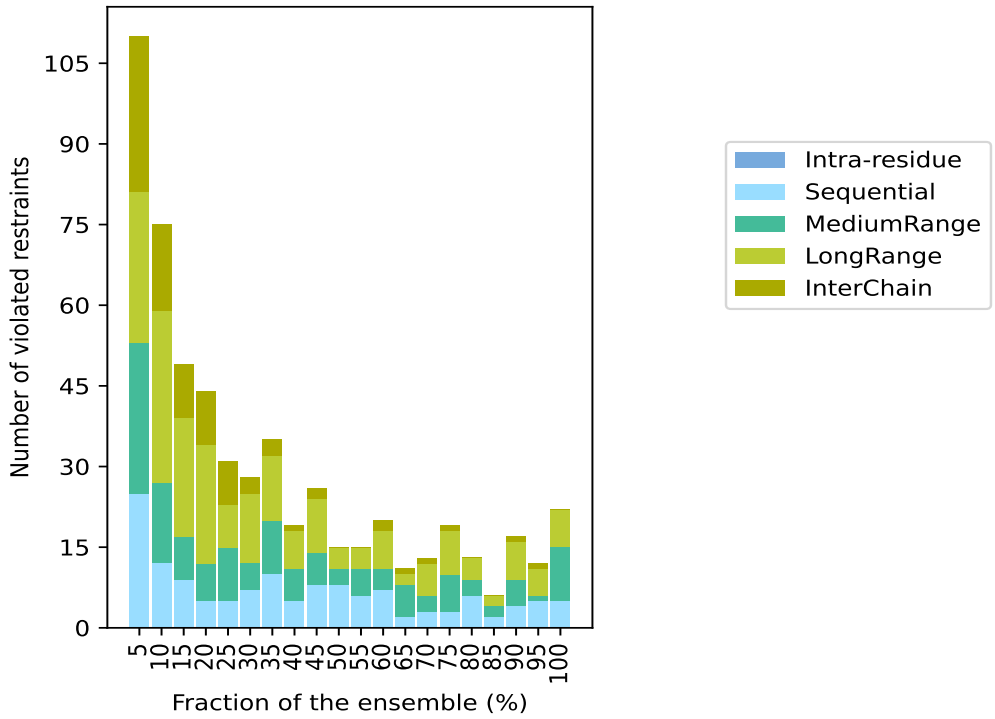
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1109(IR:0, SQ:525, MR:216, LR:310, IC:58) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	25	28	28	29	110	1	5.0
0	12	15	32	16	75	2	10.0
0	9	8	22	10	49	3	15.0
0	5	7	22	10	44	4	20.0
0	5	10	8	8	31	5	25.0
0	7	5	13	3	28	6	30.0
0	10	10	12	3	35	7	35.0
0	5	6	7	1	19	8	40.0
0	8	6	10	2	26	9	45.0
0	8	3	4	0	15	10	50.0
0	6	5	4	0	15	11	55.0
0	7	4	7	2	20	12	60.0
0	2	6	2	1	11	13	65.0
0	3	3	6	1	13	14	70.0
0	3	7	8	1	19	15	75.0
0	6	3	4	0	13	16	80.0
0	2	2	2	0	6	17	85.0
0	4	5	7	1	17	18	90.0
0	5	1	5	1	12	19	95.0
0	5	10	7	0	22	20	100.0

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

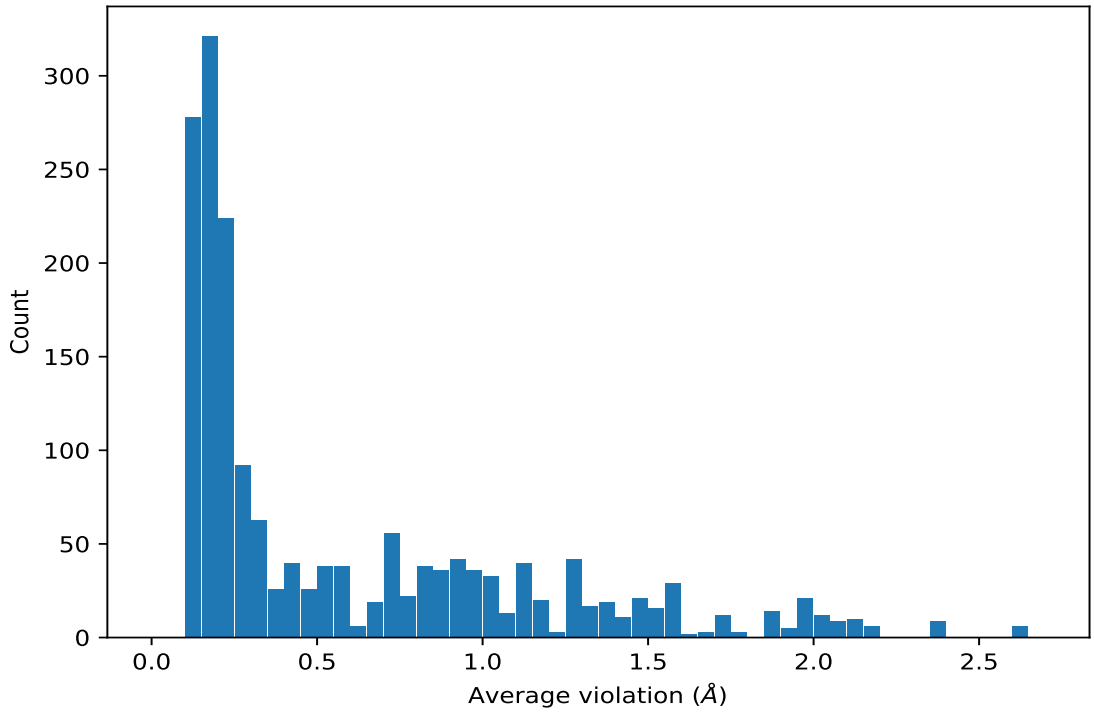
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	20	2.11	0.89	2.2
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	20	2.11	0.89	2.2
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	20	1.92	1.72	1.1
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	20	1.92	1.72	1.1
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	20	1.92	1.72	1.1
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	20	1.86	0.83	1.98
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	20	1.86	0.83	1.98
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	20	1.86	0.83	1.98
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	20	1.39	0.42	1.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	20	1.39	0.42	1.23
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	20	1.39	0.42	1.23
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	20	0.68	0.12	0.69
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	20	0.56	0.18	0.58
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	20	0.55	0.13	0.58
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	20	0.55	0.13	0.58
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	20	0.55	0.13	0.58
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	20	0.52	0.26	0.55
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	20	0.51	0.27	0.48
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	20	0.49	0.11	0.5
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	20	0.45	0.12	0.42
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	20	0.44	0.12	0.48
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	20	0.42	0.11	0.44
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	20	0.42	0.11	0.42
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	20	0.41	0.1	0.41
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	20	0.38	0.13	0.38
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	20	0.37	0.1	0.36
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	20	0.32	0.08	0.32
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	20	0.32	0.15	0.27
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	20	0.31	0.07	0.32
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	20	0.23	0.07	0.22
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	20	0.22	0.05	0.21
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	19	2.37	1.1	2.36
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	19	2.37	1.1	2.36
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	19	0.54	0.28	0.48
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	19	0.52	0.21	0.53
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	19	0.4	0.12	0.41
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	19	0.37	0.15	0.35
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	19	0.37	0.15	0.35
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	19	0.37	0.15	0.35
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	19	0.34	0.13	0.36
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	19	0.31	0.09	0.32
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	19	0.29	0.07	0.27
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	19	0.28	0.1	0.26
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	19	0.28	0.1	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	19	0.28	0.1	0.26
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	19	0.28	0.1	0.26
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	19	0.28	0.1	0.26
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	19	0.28	0.1	0.26
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	19	0.24	0.08	0.26
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	19	0.19	0.05	0.19
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	19	0.14	0.02	0.14
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	18	2.17	0.61	2.2
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	18	2.17	0.61	2.2
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	18	2.17	0.61	2.2
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	18	2.15	0.38	2.2
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	18	2.15	0.38	2.2
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	18	2.15	0.38	2.2
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	18	1.87	1.95	1.4
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	18	1.87	1.95	1.4
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	18	1.47	1.05	1.25
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	18	1.47	1.05	1.25
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	18	1.34	0.53	1.65
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	18	1.34	0.53	1.65
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	18	1.34	0.53	1.65
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	18	1.31	0.21	1.38
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	18	1.31	0.21	1.38
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	18	1.31	0.21	1.38
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	18	0.72	0.5	0.55
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	18	0.72	0.5	0.55
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	18	0.7	0.17	0.72
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	18	0.7	0.17	0.72
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	18	0.51	0.23	0.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	18	0.5	0.26	0.42
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	18	0.42	0.15	0.4
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	18	0.37	0.15	0.33
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	18	0.35	0.19	0.29
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	18	0.28	0.11	0.26
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	18	0.25	0.11	0.25
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	18	0.24	0.07	0.24
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	18	0.22	0.06	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	18	0.22	0.06	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	18	0.22	0.06	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	18	0.22	0.06	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	18	0.22	0.06	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	18	0.22	0.06	0.21
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	17	0.37	0.16	0.34
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	17	0.27	0.12	0.26
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	17	0.26	0.09	0.23
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	17	0.25	0.08	0.24
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	17	0.25	0.09	0.23
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	17	0.21	0.05	0.23
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	16	1.99	1.39	1.52
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	16	1.99	1.39	1.52
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	16	1.77	0.66	1.92
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	16	1.77	0.66	1.92
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	16	1.77	0.66	1.92
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	16	1.67	0.86	1.77
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	16	1.67	0.86	1.77
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	16	1.67	0.86	1.77
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	16	1.55	0.52	1.72
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	16	1.55	0.52	1.72
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	16	1.55	0.52	1.72
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	16	0.94	0.57	0.88
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	16	0.94	0.57	0.88
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	16	0.94	0.57	0.88
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	16	0.94	0.57	0.88
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	16	0.94	0.57	0.88

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	16	0.94	0.57	0.88
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	16	0.94	0.57	0.88
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	16	0.94	0.57	0.88
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	16	0.94	0.57	0.88
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	16	0.69	0.43	0.68
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	16	0.58	0.27	0.65
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	16	0.36	0.18	0.36
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	16	0.34	0.08	0.37
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	16	0.34	0.08	0.37
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	16	0.32	0.11	0.3
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	16	0.29	0.12	0.3
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	16	0.27	0.1	0.25
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	16	0.24	0.06	0.22
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	15	2.05	1.17	2.01
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	15	2.05	1.17	2.01
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	15	1.86	1.06	2.08
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	15	1.86	1.06	2.08
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	15	1.86	1.06	2.08
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	15	1.86	1.06	2.08
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	15	1.86	1.06	2.08
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	15	1.86	1.06	2.08
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	15	1.59	0.78	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	15	1.59	0.78	1.99
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	15	1.2	0.75	1.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	15	1.2	0.75	1.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	15	1.2	0.75	1.29
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	15	0.6	0.35	0.67
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	15	0.6	0.35	0.67

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	15	0.6	0.35	0.67
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	15	0.5	0.19	0.41
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	15	0.47	0.26	0.42
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	15	0.42	0.19	0.49
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	15	0.38	0.18	0.41
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	15	0.37	0.14	0.37
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	15	0.31	0.09	0.28
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	15	0.3	0.14	0.28
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	15	0.3	0.14	0.28
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	15	0.29	0.12	0.31
(1,679)	1:92:B:THR:H	1:94:B:MET:H	15	0.28	0.12	0.25
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	15	0.27	0.11	0.27
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	15	0.24	0.06	0.26
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	15	0.24	0.08	0.2
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	15	0.2	0.1	0.16
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	15	0.2	0.06	0.22
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	14	1.18	0.76	1.0
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	14	1.18	0.76	1.0
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	14	1.18	0.76	1.0
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	14	1.16	0.75	0.98
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	14	1.16	0.75	0.98
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	14	1.05	0.62	0.86
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	14	0.75	0.49	0.63
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	14	0.75	0.49	0.63
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	14	0.75	0.49	0.63
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	14	0.75	0.27	0.78
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	14	0.75	0.27	0.78
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	14	0.6	0.35	0.49
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	14	0.6	0.35	0.49
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	14	0.6	0.35	0.49
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	14	0.5	0.16	0.47
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	14	0.5	0.16	0.47
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	14	0.5	0.16	0.47
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	14	0.4	0.15	0.42
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	14	0.4	0.15	0.42

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	14	0.4	0.17	0.4
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	14	0.32	0.14	0.34
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	14	0.31	0.11	0.32
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	14	0.25	0.09	0.25
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	14	0.23	0.06	0.24
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	13	1.48	0.93	1.64
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	13	1.48	0.93	1.64
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	13	0.56	0.23	0.63
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	13	0.52	0.33	0.35
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	13	0.52	0.33	0.35
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	13	0.52	0.33	0.35
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	13	0.38	0.13	0.43
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	13	0.35	0.12	0.35
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	13	0.28	0.09	0.29
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	13	0.27	0.09	0.27
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	13	0.26	0.09	0.27
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	13	0.18	0.04	0.19
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	13	0.18	0.04	0.19
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	13	0.18	0.04	0.19
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	13	0.18	0.04	0.19
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	13	0.18	0.04	0.19
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	13	0.18	0.04	0.19
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	13	0.18	0.04	0.17
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	13	0.16	0.05	0.15
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	12	1.54	1.4	0.8
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	12	1.42	1.02	1.2
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	12	1.42	1.02	1.2
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	12	1.22	0.53	1.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	12	1.22	0.53	1.17
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	12	1.22	0.53	1.17
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	12	1.15	0.36	1.15
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	12	1.15	0.36	1.15
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	12	1.15	0.36	1.15
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	12	1.15	0.36	1.15
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	12	1.15	0.36	1.15
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	12	1.15	0.36	1.15
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	12	1.05	0.81	0.94
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	12	1.05	0.81	0.94
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	12	1.05	0.81	0.94
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	12	1.01	0.72	0.82
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	12	1.01	0.72	0.82
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	12	1.01	0.72	0.82
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	12	1.01	0.72	0.82
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	12	1.01	0.72	0.82
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	12	1.01	0.72	0.82
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	12	0.82	0.2	0.76
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	12	0.82	0.2	0.76
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	12	0.82	0.2	0.76
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	12	0.37	0.17	0.4
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	12	0.3	0.07	0.3
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	12	0.28	0.13	0.28
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	12	0.27	0.09	0.26
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	12	0.26	0.09	0.24
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	12	0.24	0.1	0.24
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	12	0.24	0.06	0.2
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	12	0.23	0.08	0.24
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	12	0.21	0.08	0.2
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	12	0.2	0.04	0.2
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	12	0.2	0.04	0.2
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	12	0.2	0.04	0.2
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	12	0.2	0.09	0.17
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	12	0.2	0.09	0.17
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	12	0.2	0.09	0.17
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	12	0.2	0.09	0.17
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	12	0.2	0.09	0.17
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	12	0.2	0.09	0.17
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	12	0.18	0.06	0.16
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	12	0.18	0.04	0.2
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	11	1.55	0.81	1.76
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	11	1.55	0.81	1.76

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	11	1.18	0.48	1.15
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	11	1.18	0.48	1.15
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	11	1.18	0.48	1.15
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	11	1.02	0.6	0.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	11	1.02	0.6	0.92
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	11	0.89	0.49	0.67
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	11	0.89	0.49	0.67
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	11	0.8	0.23	0.87
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	11	0.8	0.23	0.87
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	11	0.8	0.23	0.87
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	11	0.71	0.36	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	11	0.71	0.36	0.51
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	11	0.37	0.18	0.32
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	11	0.27	0.1	0.26
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	11	0.25	0.11	0.22
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	11	0.24	0.07	0.24
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	11	0.2	0.06	0.2
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	11	0.18	0.07	0.15
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	11	0.16	0.05	0.15
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	11	0.16	0.05	0.15
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	11	0.16	0.05	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	11	0.16	0.05	0.15
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	11	0.16	0.05	0.15
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	11	0.16	0.05	0.15
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	11	0.16	0.05	0.15
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	11	0.16	0.05	0.15
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	11	0.16	0.05	0.15
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	11	0.16	0.04	0.18
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	11	0.16	0.03	0.14
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	10	1.71	0.52	1.96
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	10	1.71	0.52	1.96
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	10	1.71	0.52	1.96
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	10	1.42	0.95	1.5
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	10	1.42	0.95	1.5
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	10	1.26	0.52	1.34
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	10	1.26	0.52	1.34
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	10	1.26	0.52	1.34
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	10	1.26	0.52	1.34
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	10	1.26	0.52	1.34
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	10	1.26	0.52	1.34
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	10	0.92	0.42	0.8
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	10	0.92	0.42	0.8
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	10	0.83	0.6	0.72
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	10	0.83	0.6	0.72
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	10	0.37	0.16	0.35
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	10	0.31	0.12	0.32
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	10	0.26	0.18	0.16
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	10	0.25	0.13	0.22
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	10	0.25	0.13	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	10	0.21	0.07	0.18
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	10	0.18	0.07	0.15
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	10	0.17	0.05	0.16
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	10	0.16	0.04	0.15
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	10	0.16	0.04	0.16
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	10	0.14	0.02	0.14
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	9	1.87	0.75	1.85
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	9	1.87	0.75	1.85
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	9	1.87	0.75	1.85
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	9	1.59	0.99	1.5
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	9	1.59	0.99	1.5
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	9	1.56	0.93	1.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	9	1.56	0.93	1.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	9	1.56	0.93	1.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	9	1.56	0.93	1.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	9	1.56	0.93	1.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	9	1.56	0.93	1.44
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	9	1.48	0.54	1.43
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	9	1.48	0.54	1.43
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	9	1.48	0.54	1.43
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	9	1.38	0.74	1.55
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	9	1.38	0.74	1.55
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	9	1.34	0.87	1.7
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	9	1.34	0.87	1.7
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	9	1.15	0.73	0.79
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	9	1.15	0.73	0.79
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	9	1.15	0.73	0.79
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	9	1.15	0.73	0.79

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	9	1.15	0.73	0.79
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	9	1.15	0.73	0.79
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	9	1.05	0.44	1.11
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	9	1.05	0.44	1.11
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	9	1.05	0.44	1.11
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	9	1.03	0.64	0.77
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	9	1.03	0.64	0.77
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	9	0.8	0.34	0.85
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	9	0.8	0.34	0.85
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	9	0.45	0.17	0.48
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	9	0.45	0.17	0.48
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	9	0.39	0.19	0.39
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	9	0.37	0.16	0.37
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	9	0.37	0.16	0.37
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	9	0.37	0.16	0.37
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	9	0.31	0.1	0.3
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	9	0.27	0.05	0.27
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	9	0.27	0.05	0.27
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	9	0.27	0.05	0.27
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	9	0.23	0.08	0.23
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	9	0.19	0.07	0.2
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	9	0.18	0.03	0.18
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	9	0.18	0.05	0.16
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	9	0.17	0.05	0.15
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	9	0.17	0.04	0.18
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	9	0.17	0.03	0.18
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	9	0.17	0.06	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	9	0.17	0.06	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	9	0.17	0.06	0.15
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	9	0.17	0.05	0.16
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	9	0.16	0.04	0.16
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	9	0.15	0.05	0.14
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	9	0.15	0.05	0.14
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	9	0.15	0.05	0.14
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	8	1.97	1.02	2.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	8	1.97	1.02	2.2
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	8	1.97	1.02	2.2
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	8	1.35	0.37	1.4
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	8	1.35	0.37	1.4
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	8	1.35	0.37	1.4
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	8	1.27	1.06	1.02
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	8	1.27	1.06	1.02
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	8	0.99	0.57	0.88
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	8	0.99	0.57	0.88
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	8	0.86	1.16	0.48
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	8	0.86	1.16	0.48
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	8	0.72	0.22	0.66
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	8	0.72	0.22	0.66
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	8	0.72	0.22	0.66
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	8	0.66	0.37	0.66
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	8	0.66	0.37	0.66
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	8	0.66	0.37	0.66
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	8	0.57	0.13	0.59
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	8	0.57	0.13	0.59
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	8	0.52	0.31	0.44
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	8	0.52	0.31	0.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	8	0.52	0.31	0.44
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	8	0.52	0.31	0.44
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	8	0.52	0.31	0.44
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	8	0.52	0.31	0.44
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	8	0.52	0.31	0.44
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	8	0.52	0.31	0.44
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	8	0.52	0.31	0.44
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	8	0.37	0.17	0.3
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	8	0.31	0.12	0.27
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	8	0.3	0.11	0.32
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	8	0.27	0.15	0.24
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	8	0.27	0.15	0.24
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	8	0.27	0.15	0.24
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	8	0.2	0.12	0.16
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	8	0.2	0.07	0.22
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	8	0.18	0.05	0.18
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	8	0.17	0.09	0.14
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	8	0.16	0.04	0.16
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	8	0.16	0.04	0.16
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	8	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	8	0.15	0.04	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	8	0.15	0.04	0.14
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	7	2.05	0.63	2.29
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	7	2.05	0.63	2.29
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	7	2.05	0.63	2.29
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	7	1.98	0.39	2.12
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	7	1.98	0.39	2.12
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	7	1.98	0.39	2.12
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	7	1.95	1.89	0.59
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	7	1.95	1.89	0.59
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	7	1.65	0.64	1.9
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	7	1.61	1.05	1.38
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	7	1.39	0.81	1.62
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	7	1.35	0.9	1.19
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	7	1.35	0.9	1.19
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	7	1.35	0.9	1.19
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	7	1.32	0.6	1.43
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	7	1.32	0.6	1.43
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	7	1.13	0.66	0.89
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	7	1.08	0.37	1.24
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	7	1.08	0.37	1.24
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	7	1.08	0.37	1.24
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	7	0.98	0.59	1.01
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	7	0.98	0.59	1.01

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	7	0.98	0.59	1.01
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	7	0.98	0.59	1.01
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	7	0.98	0.59	1.01
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	7	0.98	0.59	1.01
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	7	0.98	0.59	1.01
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	7	0.98	0.59	1.01
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	7	0.98	0.59	1.01
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	7	0.58	0.27	0.49
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	7	0.58	0.27	0.49
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	7	0.45	0.13	0.41
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	7	0.45	0.13	0.41
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	7	0.43	0.24	0.29
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	7	0.43	0.24	0.29
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	7	0.43	0.26	0.41
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	7	0.42	0.16	0.43
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	7	0.42	0.16	0.43
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	7	0.42	0.16	0.43
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	7	0.37	0.23	0.3
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	7	0.33	0.16	0.39
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	7	0.32	0.16	0.28
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	7	0.31	0.18	0.2
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	7	0.25	0.1	0.22
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	7	0.25	0.1	0.22
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	7	0.25	0.07	0.24
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	7	0.24	0.11	0.2
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	7	0.24	0.11	0.2
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	7	0.24	0.13	0.2
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	7	0.24	0.06	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	7	0.23	0.07	0.22
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	7	0.23	0.09	0.22
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	7	0.2	0.04	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	7	0.2	0.04	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	7	0.2	0.04	0.19
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	7	0.19	0.06	0.19
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	7	0.18	0.03	0.18
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	7	0.16	0.05	0.14
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	7	0.16	0.03	0.15
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	7	0.15	0.02	0.16
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	7	0.15	0.09	0.11
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	7	0.15	0.09	0.11
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	7	0.15	0.09	0.11
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	7	0.15	0.09	0.11
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	7	0.15	0.09	0.11
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	7	0.15	0.09	0.11
(1,359)	1:122:A:THR:H	1:18:B:THR:H	7	0.15	0.03	0.13
(1,476)	1:36:B:TRP:HZ3	1:37:B:GLN:H	6	2.1	0.18	2.14
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD21	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD22	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD23	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD21	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD22	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD23	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD21	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD22	6	2.07	0.93	1.99
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD23	6	2.07	0.93	1.99
(1,1278)	1:36:D:TRP:HZ3	1:37:D:GLN:H	6	1.74	0.78	1.9
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD11	6	1.03	0.55	0.94
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD12	6	1.03	0.55	0.94
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD13	6	1.03	0.55	0.94
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD11	6	1.03	0.55	0.94
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD12	6	1.03	0.55	0.94
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD13	6	1.03	0.55	0.94
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG21	6	0.9	0.36	0.92
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG22	6	0.9	0.36	0.92
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG23	6	0.9	0.36	0.92
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG21	6	0.9	0.36	0.92
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG22	6	0.9	0.36	0.92
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG23	6	0.9	0.36	0.92
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG21	6	0.9	0.36	0.92
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG22	6	0.9	0.36	0.92

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG23	6	0.9	0.36	0.92
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE1	6	0.86	0.54	0.76
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE2	6	0.86	0.54	0.76
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE3	6	0.86	0.54	0.76
(1,686)	1:94:B:MET:HE1	1:95:B:ALA:H	6	0.81	0.51	0.73
(1,686)	1:94:B:MET:HE2	1:95:B:ALA:H	6	0.81	0.51	0.73
(1,686)	1:94:B:MET:HE3	1:95:B:ALA:H	6	0.81	0.51	0.73
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD11	6	0.79	0.33	0.88
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD12	6	0.79	0.33	0.88
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD13	6	0.79	0.33	0.88
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD11	6	0.79	0.33	0.88
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD12	6	0.79	0.33	0.88
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD13	6	0.79	0.33	0.88
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	6	0.59	0.29	0.65
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	6	0.59	0.29	0.65
(1,888)	1:39:C:GLU:H	1:67:C:SER:H	6	0.51	0.2	0.5
(1,177)	1:59:A:VAL:HG11	1:81:A:GLY:H	6	0.34	0.18	0.29
(1,177)	1:59:A:VAL:HG12	1:81:A:GLY:H	6	0.34	0.18	0.29
(1,177)	1:59:A:VAL:HG13	1:81:A:GLY:H	6	0.34	0.18	0.29
(1,532)	1:49:B:SER:H	1:59:B:VAL:H	6	0.34	0.13	0.34
(1,908)	1:43:C:ASP:H	1:63:C:THR:H	6	0.31	0.14	0.28
(1,176)	1:59:A:VAL:HG11	1:80:A:GLN:H	6	0.26	0.1	0.24
(1,176)	1:59:A:VAL:HG12	1:80:A:GLN:H	6	0.26	0.1	0.24
(1,176)	1:59:A:VAL:HG13	1:80:A:GLN:H	6	0.26	0.1	0.24
(1,899)	1:41:C:LYS:H	1:67:C:SER:H	6	0.26	0.12	0.28
(1,131)	1:47:A:ALA:H	1:61:A:ARG:H	6	0.24	0.12	0.22
(1,180)	1:59:A:VAL:HG21	1:82:A:GLY:H	6	0.24	0.09	0.24
(1,180)	1:59:A:VAL:HG22	1:82:A:GLY:H	6	0.24	0.09	0.24
(1,180)	1:59:A:VAL:HG23	1:82:A:GLY:H	6	0.24	0.09	0.24
(1,595)	1:64:B:VAL:H	1:76:B:CYS:H	6	0.22	0.06	0.22
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB1	6	0.22	0.07	0.24
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB2	6	0.22	0.07	0.24
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB3	6	0.22	0.07	0.24
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG11	6	0.2	0.09	0.17
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG12	6	0.2	0.09	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG13	6	0.2	0.09	0.17
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG11	6	0.2	0.09	0.17
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG12	6	0.2	0.09	0.17
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG13	6	0.2	0.09	0.17
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG11	6	0.2	0.09	0.17
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG12	6	0.2	0.09	0.17
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG13	6	0.2	0.09	0.17
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG11	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG12	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG13	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG11	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG12	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG13	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG11	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG12	6	0.19	0.07	0.16
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG13	6	0.19	0.07	0.16
(1,697)	1:97:B:CYS:H	1:99:B:GLY:H	6	0.18	0.06	0.17
(1,66)	1:28:A:ALA:H	1:30:A:HIS:H	6	0.17	0.06	0.15
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE1	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE2	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE3	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE1	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE2	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE3	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE1	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE2	6	0.17	0.07	0.14
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE3	6	0.17	0.07	0.14
(1,395)	1:140:A:TYR:H	1:141:A:LEU:H	6	0.15	0.03	0.16
(1,266)	1:85:A:SER:H	1:86:A:ILE:H	6	0.15	0.04	0.14
(1,1073)	1:87:C:ALA:H	1:88:C:GLY:H	6	0.15	0.03	0.16
(1,410)	1:12:B:GLN:H	1:13:B:ILE:H	6	0.13	0.02	0.12
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD21	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD22	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD23	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD21	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD22	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD23	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD21	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD22	5	1.29	1.08	0.79
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD23	5	1.29	1.08	0.79
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD21	5	1.12	0.63	0.88
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD22	5	1.12	0.63	0.88

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD23	5	1.12	0.63	0.88
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD21	5	1.12	0.63	0.88
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD22	5	1.12	0.63	0.88
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD23	5	1.12	0.63	0.88
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD21	5	1.12	0.63	0.88
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD22	5	1.12	0.63	0.88
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD23	5	1.12	0.63	0.88
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG21	5	1.0	0.21	0.98
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG22	5	1.0	0.21	0.98
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG23	5	1.0	0.21	0.98
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG11	5	0.64	0.15	0.58
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG12	5	0.64	0.15	0.58
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG13	5	0.64	0.15	0.58
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD21	5	0.46	0.23	0.59
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD22	5	0.46	0.23	0.59
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD23	5	0.46	0.23	0.59
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD21	5	0.46	0.23	0.59
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD22	5	0.46	0.23	0.59
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD23	5	0.46	0.23	0.59
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD1	5	0.35	0.19	0.27
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD2	5	0.35	0.19	0.27
(1,1189)	1:137:C:PHE:H	1:140:C:TYR:H	5	0.32	0.22	0.22
(1,1495)	1:100:D:ALA:H	1:102:D:CYS:H	5	0.28	0.09	0.27
(1,289)	1:95:A:ALA:H	1:98:A:LEU:H	5	0.25	0.12	0.27
(1,1090)	1:94:C:MET:H	1:96:C:HIS:H	5	0.25	0.11	0.17
(1,103)	1:41:A:LYS:H	1:65:A:THR:H	5	0.21	0.06	0.23
(1,335)	1:114:A:ILE:H	1:117:A:MET:H	5	0.21	0.04	0.22
(1,1094)	1:95:C:ALA:H	1:98:C:LEU:H	5	0.21	0.11	0.18
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE1	5	0.21	0.14	0.14
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE2	5	0.21	0.14	0.14
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE1	5	0.21	0.14	0.14
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE2	5	0.21	0.14	0.14
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE1	5	0.21	0.14	0.14
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE2	5	0.21	0.14	0.14
(1,1030)	1:68:C:LEU:H	1:73:C:ALA:H	5	0.2	0.04	0.2
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG11	5	0.2	0.07	0.17
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG12	5	0.2	0.07	0.17
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG13	5	0.2	0.07	0.17
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG11	5	0.2	0.07	0.17
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG12	5	0.2	0.07	0.17
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG13	5	0.2	0.07	0.17
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG11	5	0.2	0.07	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG12	5	0.2	0.07	0.17
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG13	5	0.2	0.07	0.17
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD11	5	0.2	0.05	0.23
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD12	5	0.2	0.05	0.23
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD13	5	0.2	0.05	0.23
(1,866)	1:30:C:HIS:H	1:32:C:PHE:H	5	0.19	0.06	0.2
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD11	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD12	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD13	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD11	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD12	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD13	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD11	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD12	5	0.19	0.06	0.16
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD13	5	0.19	0.06	0.16
(1,885)	1:36:C:TRP:H	1:37:C:GLN:H	5	0.18	0.07	0.2
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD11	5	0.17	0.05	0.16
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD12	5	0.17	0.05	0.16
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD13	5	0.17	0.05	0.16
(1,1055)	1:77:C:GLU:H	1:78:C:VAL:H	5	0.17	0.03	0.17
(1,354)	1:119:A:SER:H	1:123:A:PHE:H	5	0.16	0.05	0.15
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG11	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG12	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG13	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG11	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG12	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG13	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG11	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG12	5	0.16	0.05	0.17
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG13	5	0.16	0.05	0.17
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB1	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB2	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB3	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB1	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB2	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB3	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB1	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB2	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB3	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB1	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB2	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB3	5	0.16	0.06	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB1	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB2	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB3	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB1	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB2	5	0.16	0.06	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB3	5	0.16	0.06	0.12
(1,985)	1:60:C:LEU:H	1:81:C:GLY:H	5	0.15	0.05	0.12
(1,1313)	1:46:D:THR:H	1:61:D:ARG:H	5	0.15	0.04	0.14
(1,844)	1:22:C:SER:H	1:23:D:PHE:H	5	0.15	0.04	0.13
(1,1271)	1:35:D:ASP:H	1:36:D:TRP:H	5	0.14	0.03	0.13
(1,1506)	1:110:D:ALA:H	1:112:D:GLU:H	5	0.13	0.02	0.12
(1,522)	1:47:B:ALA:H	1:48:B:SER:H	5	0.12	0.01	0.12
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	4	1.74	2.1	0.7
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	4	1.74	2.1	0.7
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	4	1.74	2.1	0.7
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	4	1.74	2.1	0.7
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	4	1.74	2.1	0.7
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	4	1.74	2.1	0.7
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD11	4	1.54	0.61	1.52
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD12	4	1.54	0.61	1.52
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD13	4	1.54	0.61	1.52
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD11	4	1.54	0.61	1.52
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD12	4	1.54	0.61	1.52
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD13	4	1.54	0.61	1.52
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD21	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD22	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD23	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD21	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD22	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD23	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD21	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD22	4	1.27	0.64	1.4
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD23	4	1.27	0.64	1.4
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB1	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB2	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB3	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB1	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB2	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB3	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB1	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB2	4	1.15	0.49	1.31
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB3	4	1.15	0.49	1.31

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG11	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG12	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG13	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG11	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG12	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG13	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG11	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG12	4	1.12	0.41	1.05
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG13	4	1.12	0.41	1.05
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD11	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD12	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD13	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD11	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD12	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD13	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD11	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD12	4	0.99	0.67	0.97
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD13	4	0.99	0.67	0.97
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD11	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD12	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD13	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD11	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD12	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD13	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD11	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD12	4	0.97	0.49	0.94
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD13	4	0.97	0.49	0.94
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG11	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG12	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG13	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG11	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG12	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG13	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG11	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG12	4	0.89	0.67	0.8
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG13	4	0.89	0.67	0.8
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE1	4	0.77	0.18	0.76
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE2	4	0.77	0.18	0.76
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD11	4	0.71	0.28	0.64
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD12	4	0.71	0.28	0.64
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD13	4	0.71	0.28	0.64
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD11	4	0.71	0.28	0.64

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD12	4	0.71	0.28	0.64
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD13	4	0.71	0.28	0.64
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD11	4	0.71	0.28	0.64
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD12	4	0.71	0.28	0.64
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD13	4	0.71	0.28	0.64
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE1	4	0.67	0.55	0.48
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE2	4	0.67	0.55	0.48
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE3	4	0.67	0.55	0.48
(1,348)	1:118:A:VAL:HG11	1:123:A:PHE:H	4	0.54	0.08	0.53
(1,348)	1:118:A:VAL:HG12	1:123:A:PHE:H	4	0.54	0.08	0.53
(1,348)	1:118:A:VAL:HG13	1:123:A:PHE:H	4	0.54	0.08	0.53
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	4	0.4	0.13	0.4
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	4	0.4	0.13	0.4
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	4	0.4	0.13	0.4
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	4	0.4	0.13	0.4
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD21	4	0.38	0.2	0.41
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD22	4	0.38	0.2	0.41
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD23	4	0.38	0.2	0.41
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	4	0.34	0.1	0.33
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	4	0.34	0.1	0.33
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD21	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD22	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD23	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD21	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD22	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD23	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD21	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD22	4	0.34	0.21	0.22
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD23	4	0.34	0.21	0.22
(1,1467)	1:92:D:THR:H	1:95:D:ALA:H	4	0.28	0.11	0.24
(1,1334)	1:51:D:LEU:H	1:57:D:GLU:H	4	0.27	0.05	0.25
(1,1201)	1:10:D:THR:H	1:87:D:ALA:H	4	0.26	0.12	0.26
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG11	4	0.25	0.13	0.24
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG12	4	0.25	0.13	0.24
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG13	4	0.25	0.13	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG11	4	0.25	0.13	0.24
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG12	4	0.25	0.13	0.24
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG13	4	0.25	0.13	0.24
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG11	4	0.25	0.13	0.24
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG12	4	0.25	0.13	0.24
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG13	4	0.25	0.13	0.24
(1,221)	1:67:A:SER:H	1:73:A:ALA:H	4	0.24	0.06	0.24
(1,1472)	1:94:D:MET:H	1:96:D:HIS:H	4	0.23	0.06	0.22
(1,179)	1:59:A:VAL:HG21	1:81:A:GLY:H	4	0.22	0.16	0.12
(1,179)	1:59:A:VAL:HG22	1:81:A:GLY:H	4	0.22	0.16	0.12
(1,179)	1:59:A:VAL:HG23	1:81:A:GLY:H	4	0.22	0.16	0.12
(1,934)	1:49:C:SER:H	1:57:C:GLU:H	4	0.21	0.05	0.21
(1,961)	1:55:C:VAL:H	1:86:C:ILE:H	4	0.2	0.07	0.17
(1,1490)	1:99:D:GLY:H	1:100:D:ALA:H	4	0.2	0.07	0.18
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB1	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB2	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB3	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB1	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB2	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB3	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB1	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB2	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB3	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB1	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB2	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB3	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB1	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB2	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB3	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB1	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB2	4	0.2	0.01	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB3	4	0.2	0.01	0.2
(1,1414)	1:68:D:LEU:H	1:71:D:GLU:H	4	0.2	0.1	0.15
(1,474)	1:36:B:TRP:HE1	1:37:B:GLN:H	4	0.18	0.01	0.18
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG11	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG12	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG13	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG21	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG22	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG23	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG11	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG12	4	0.18	0.04	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG13	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG21	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG22	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG23	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG11	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG12	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG13	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG21	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG22	4	0.18	0.04	0.19
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG23	4	0.18	0.04	0.19
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD11	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD12	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD13	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD11	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD12	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD13	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD11	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD12	4	0.18	0.06	0.16
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD13	4	0.18	0.06	0.16
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD11	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD12	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD13	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD21	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD22	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD23	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD11	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD12	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD13	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD21	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD22	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD23	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD11	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD12	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD13	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD21	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD22	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD23	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD11	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD12	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD13	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD21	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD22	4	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD23	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD11	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD12	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD13	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD21	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD22	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD23	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD11	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD12	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD13	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD21	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD22	4	0.18	0.04	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD23	4	0.18	0.04	0.18
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG11	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG12	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG13	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG11	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG12	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG13	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG11	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG12	4	0.18	0.03	0.18
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG13	4	0.18	0.03	0.18
(1,18)	1:14:A:GLN:H	1:83:A:ILE:H	4	0.17	0.06	0.16
(1,1103)	1:97:C:CYS:H	1:100:C:ALA:H	4	0.16	0.03	0.18
(1,533)	1:50:B:GLN:H	1:51:B:LEU:H	4	0.16	0.03	0.16
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG21	4	0.16	0.04	0.16
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG22	4	0.16	0.04	0.16
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG23	4	0.16	0.04	0.16
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG21	4	0.16	0.04	0.16
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG22	4	0.16	0.04	0.16
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG23	4	0.16	0.04	0.16
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD11	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD12	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD13	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD21	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD22	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD23	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD11	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD12	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD13	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD21	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD22	4	0.16	0.05	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD23	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD11	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD12	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD13	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD21	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD22	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD23	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD11	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD12	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD13	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD21	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD22	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD23	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD11	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD12	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD13	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD21	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD22	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD23	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD11	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD12	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD13	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD21	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD22	4	0.16	0.05	0.14
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD23	4	0.16	0.05	0.14
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD11	4	0.15	0.03	0.16
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD12	4	0.15	0.03	0.16
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD13	4	0.15	0.03	0.16
(1,1540)	1:126:D:LEU:H	1:127:D:ASN:H	4	0.15	0.03	0.14
(1,222)	1:68:A:LEU:H	1:69:A:GLY:H	4	0.14	0.03	0.13
(1,356)	1:121:A:GLY:H	1:123:A:PHE:H	4	0.14	0.03	0.12
(1,308)	1:99:A:GLY:H	1:101:A:TYR:H	4	0.12	0.02	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG21	4	0.12	0.01	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG22	4	0.12	0.01	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG23	4	0.12	0.01	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG21	4	0.12	0.01	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG22	4	0.12	0.01	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG23	4	0.12	0.01	0.12
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE1	3	2.62	2.91	0.62
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE2	3	2.62	2.91	0.62
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE1	3	2.62	2.91	0.62
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE2	3	2.62	2.91	0.62

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE1	3	2.62	2.91	0.62
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE2	3	2.62	2.91	0.62
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD21	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD22	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD23	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD21	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD22	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD23	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD21	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD22	3	1.53	0.53	1.89
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD23	3	1.53	0.53	1.89
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	3	0.9	0.1	0.92
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	3	0.9	0.1	0.92
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	3	0.9	0.1	0.92
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	3	0.9	0.1	0.92
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	3	0.9	0.1	0.92
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	3	0.9	0.1	0.92
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	3	0.87	0.09	0.81
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	3	0.87	0.09	0.81
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	3	0.87	0.09	0.81
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	3	0.87	0.09	0.81
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	3	0.87	0.09	0.81
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	3	0.87	0.09	0.81
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE1	3	0.84	0.45	0.99
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE2	3	0.84	0.45	0.99
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE3	3	0.84	0.45	0.99
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG21	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG22	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG23	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG21	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG22	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG23	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG21	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG22	3	0.8	0.41	0.91
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG23	3	0.8	0.41	0.91
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG11	3	0.74	0.4	0.89
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG12	3	0.74	0.4	0.89
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG13	3	0.74	0.4	0.89
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG11	3	0.74	0.4	0.89
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG12	3	0.74	0.4	0.89
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG13	3	0.74	0.4	0.89
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG11	3	0.74	0.4	0.89

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG12	3	0.74	0.4	0.89
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG13	3	0.74	0.4	0.89
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE1	3	0.74	0.33	0.94
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE2	3	0.74	0.33	0.94
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE3	3	0.74	0.33	0.94
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE1	3	0.74	0.33	0.94
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE2	3	0.74	0.33	0.94
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE3	3	0.74	0.33	0.94
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD11	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD12	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD13	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD11	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD12	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD13	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD11	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD12	3	0.68	0.03	0.7
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD13	3	0.68	0.03	0.7
(1,1169)	1:131:C:VAL:HG11	1:133:C:PHE:H	3	0.62	0.12	0.67
(1,1169)	1:131:C:VAL:HG12	1:133:C:PHE:H	3	0.62	0.12	0.67
(1,1169)	1:131:C:VAL:HG13	1:133:C:PHE:H	3	0.62	0.12	0.67
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD11	3	0.5	0.27	0.63
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD12	3	0.5	0.27	0.63
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD13	3	0.5	0.27	0.63
(1,164)	1:56:A:TYR:H	1:86:A:ILE:H	3	0.47	0.29	0.35
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD21	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD22	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD23	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD21	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD22	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD23	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD21	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD22	3	0.41	0.03	0.4
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD23	3	0.41	0.03	0.4
(1,1107)	1:98:C:LEU:H	1:101:C:TYR:H	3	0.35	0.16	0.29
(1,1282)	1:39:D:GLU:H	1:67:D:SER:H	3	0.33	0.1	0.38
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD11	3	0.29	0.05	0.29
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD12	3	0.29	0.05	0.29
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD13	3	0.29	0.05	0.29
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD11	3	0.29	0.05	0.29
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD12	3	0.29	0.05	0.29
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD13	3	0.29	0.05	0.29
(1,305)	1:98:A:LEU:HD11	1:99:A:GLY:H	3	0.28	0.08	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,305)	1:98:A:LEU:HD12	1:99:A:GLY:H	3	0.28	0.08	0.3
(1,305)	1:98:A:LEU:HD13	1:99:A:GLY:H	3	0.28	0.08	0.3
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD21	3	0.27	0.08	0.27
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD22	3	0.27	0.08	0.27
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD23	3	0.27	0.08	0.27
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD21	3	0.27	0.08	0.27
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD22	3	0.27	0.08	0.27
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD23	3	0.27	0.08	0.27
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG11	3	0.26	0.1	0.25
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG12	3	0.26	0.1	0.25
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG13	3	0.26	0.1	0.25
(1,921)	1:45:C:ASP:H	1:63:C:THR:H	3	0.26	0.1	0.21
(1,1178)	1:134:C:ASP:H	1:136:C:LEU:H	3	0.24	0.1	0.18
(1,39)	1:19:A:LYS:H	1:79:A:GLN:H	3	0.23	0.06	0.27
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD11	3	0.23	0.0	0.23
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD12	3	0.23	0.0	0.23
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD13	3	0.23	0.0	0.23
(1,790)	1:9:C:MET:H	1:10:C:THR:H	3	0.22	0.09	0.27
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG11	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG12	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG13	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG21	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG22	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG23	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG11	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG12	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG13	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG21	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG22	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG23	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG11	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG12	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG13	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG21	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG22	3	0.21	0.13	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG23	3	0.21	0.13	0.13
(1,1471)	1:94:D:MET:H	1:95:D:ALA:H	3	0.21	0.05	0.2
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE1	3	0.2	0.07	0.23
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE2	3	0.2	0.07	0.23
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE3	3	0.2	0.07	0.23
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE1	3	0.2	0.07	0.23
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE2	3	0.2	0.07	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE3	3	0.2	0.07	0.23
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE1	3	0.2	0.07	0.23
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE2	3	0.2	0.07	0.23
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE3	3	0.2	0.07	0.23
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD11	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD12	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD13	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD11	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD12	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD13	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD11	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD12	3	0.2	0.06	0.16
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD13	3	0.2	0.06	0.16
(1,183)	1:60:A:LEU:H	1:82:A:GLY:H	3	0.2	0.07	0.19
(1,685)	1:94:B:MET:H	1:97:B:CYS:H	3	0.2	0.08	0.17
(1,965)	1:56:C:TYR:H	1:84:C:PHE:H	3	0.2	0.07	0.24
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG11	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG12	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG13	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG11	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG12	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG13	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG11	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG12	3	0.2	0.08	0.15
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG13	3	0.2	0.08	0.15
(1,708)	1:100:B:ALA:H	1:101:B:TYR:H	3	0.18	0.03	0.18
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD1	3	0.17	0.05	0.14
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD2	3	0.17	0.05	0.14
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD1	3	0.17	0.05	0.14
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD2	3	0.17	0.05	0.14
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD1	3	0.17	0.05	0.14
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD2	3	0.17	0.05	0.14
(1,767)	1:134:B:ASP:H	1:136:B:LEU:H	3	0.16	0.03	0.17
(1,528)	1:48:B:SER:H	1:59:B:VAL:H	3	0.16	0.04	0.13
(1,941)	1:51:C:LEU:H	1:52:C:ALA:H	3	0.15	0.03	0.13
(1,895)	1:41:C:LYS:H	1:42:C:LEU:H	3	0.15	0.01	0.14
(1,684)	1:94:B:MET:H	1:96:B:HIS:H	3	0.15	0.03	0.15
(1,1208)	1:12:D:GLN:H	1:85:D:SER:H	3	0.15	0.02	0.15
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB1	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB2	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB3	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB1	3	0.15	0.02	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB2	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB3	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB1	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB2	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB3	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB1	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB2	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB3	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB1	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB2	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB3	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB1	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB2	3	0.15	0.02	0.16
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB3	3	0.15	0.02	0.16
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD1	3	0.15	0.02	0.14
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD2	3	0.15	0.02	0.14
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD1	3	0.15	0.02	0.14
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD2	3	0.15	0.02	0.14
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD1	3	0.15	0.02	0.14
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD2	3	0.15	0.02	0.14
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE1	3	0.15	0.06	0.11
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE2	3	0.15	0.06	0.11
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE1	3	0.15	0.06	0.11
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE2	3	0.15	0.06	0.11
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE1	3	0.15	0.06	0.11
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE2	3	0.15	0.06	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB1	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB2	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB3	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB1	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB2	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB3	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB1	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB2	3	0.14	0.05	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB3	3	0.14	0.05	0.11
(1,293)	1:96:A:HIS:H	1:97:A:CYS:H	3	0.13	0.01	0.13
(1,535)	1:51:B:LEU:H	1:52:B:ALA:H	3	0.13	0.02	0.12
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD11	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD12	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD13	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD21	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD22	3	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD23	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD11	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD12	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD13	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD21	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD22	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD23	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD11	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD12	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD13	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD21	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD22	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD23	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD11	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD12	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD13	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD21	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD22	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD23	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD11	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD12	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD13	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD21	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD22	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD23	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD11	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD12	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD13	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD21	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD22	3	0.13	0.02	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD23	3	0.13	0.02	0.14
(1,995)	1:62:C:VAL:H	1:63:C:THR:H	3	0.12	0.0	0.12
(1,139)	1:50:A:GLN:H	1:57:A:GLU:H	3	0.11	0.0	0.11
(1,1549)	1:131:D:VAL:HG11	1:133:D:PHE:HE1	2	1.98	0.46	1.98
(1,1549)	1:131:D:VAL:HG11	1:133:D:PHE:HE2	2	1.98	0.46	1.98
(1,1549)	1:131:D:VAL:HG12	1:133:D:PHE:HE1	2	1.98	0.46	1.98
(1,1549)	1:131:D:VAL:HG12	1:133:D:PHE:HE2	2	1.98	0.46	1.98
(1,1549)	1:131:D:VAL:HG13	1:133:D:PHE:HE1	2	1.98	0.46	1.98
(1,1549)	1:131:D:VAL:HG13	1:133:D:PHE:HE2	2	1.98	0.46	1.98
(1,939)	1:50:C:GLN:H	1:56:C:TYR:HE1	2	1.74	1.56	1.74
(1,939)	1:50:C:GLN:H	1:56:C:TYR:HE2	2	1.74	1.56	1.74
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD11	2	1.29	1.12	1.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD12	2	1.29	1.12	1.29
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD13	2	1.29	1.12	1.29
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD11	2	1.29	1.12	1.29
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD12	2	1.29	1.12	1.29
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD13	2	1.29	1.12	1.29
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD11	2	1.29	1.12	1.29
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD12	2	1.29	1.12	1.29
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD13	2	1.29	1.12	1.29
(1,938)	1:50:C:GLN:H	1:56:C:TYR:HD1	2	1.17	1.01	1.17
(1,938)	1:50:C:GLN:H	1:56:C:TYR:HD2	2	1.17	1.01	1.17
(1,367)	1:131:A:VAL:HG11	1:133:A:PHE:H	2	1.06	0.09	1.06
(1,367)	1:131:A:VAL:HG12	1:133:A:PHE:H	2	1.06	0.09	1.06
(1,367)	1:131:A:VAL:HG13	1:133:A:PHE:H	2	1.06	0.09	1.06
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	2	0.94	0.45	0.94
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	2	0.94	0.45	0.94
(1,349)	1:118:A:VAL:HG11	1:123:A:PHE:HD1	2	0.84	0.04	0.84
(1,349)	1:118:A:VAL:HG11	1:123:A:PHE:HD2	2	0.84	0.04	0.84
(1,349)	1:118:A:VAL:HG12	1:123:A:PHE:HD1	2	0.84	0.04	0.84
(1,349)	1:118:A:VAL:HG12	1:123:A:PHE:HD2	2	0.84	0.04	0.84
(1,349)	1:118:A:VAL:HG13	1:123:A:PHE:HD1	2	0.84	0.04	0.84
(1,349)	1:118:A:VAL:HG13	1:123:A:PHE:HD2	2	0.84	0.04	0.84
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD21	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD22	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD23	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD21	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD22	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD23	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD21	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD22	2	0.79	0.12	0.79
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD23	2	0.79	0.12	0.79
(1,945)	1:51:C:LEU:H	1:56:C:TYR:HD1	2	0.74	0.56	0.74
(1,945)	1:51:C:LEU:H	1:56:C:TYR:HD2	2	0.74	0.56	0.74
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD11	2	0.72	0.5	0.72
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD12	2	0.72	0.5	0.72
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD13	2	0.72	0.5	0.72

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD11	2	0.72	0.5	0.72
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD12	2	0.72	0.5	0.72
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD13	2	0.72	0.5	0.72
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD11	2	0.72	0.5	0.72
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD12	2	0.72	0.5	0.72
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD13	2	0.72	0.5	0.72
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD11	2	0.6	0.02	0.6
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD12	2	0.6	0.02	0.6
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD13	2	0.6	0.02	0.6
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD11	2	0.6	0.02	0.6
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD12	2	0.6	0.02	0.6
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD13	2	0.6	0.02	0.6
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD21	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD22	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD23	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD21	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD22	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD23	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD21	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD22	2	0.51	0.22	0.51
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD23	2	0.51	0.22	0.51
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD21	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD22	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD23	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD21	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD22	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD23	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD21	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD22	2	0.49	0.24	0.49
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD23	2	0.49	0.24	0.49
(1,122)	1:44:A:LEU:HD21	1:45:A:ASP:H	2	0.45	0.34	0.45
(1,122)	1:44:A:LEU:HD22	1:45:A:ASP:H	2	0.45	0.34	0.45
(1,122)	1:44:A:LEU:HD23	1:45:A:ASP:H	2	0.45	0.34	0.45
(1,5)	1:11:A:PHE:HD1	1:12:A:GLN:H	2	0.41	0.17	0.41
(1,5)	1:11:A:PHE:HD2	1:12:A:GLN:H	2	0.41	0.17	0.41
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	2	0.4	0.19	0.4
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	2	0.4	0.19	0.4
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	2	0.4	0.19	0.4
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	2	0.4	0.19	0.4
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	2	0.4	0.19	0.4
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	2	0.4	0.19	0.4
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	2	0.4	0.19	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	2	0.4	0.19	0.4
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	2	0.4	0.19	0.4
(1,1182)	1:135:C:ALA:H	1:138:C:MET:H	2	0.38	0.16	0.38
(1,1569)	1:137:D:PHE:H	1:140:D:TYR:H	2	0.36	0.06	0.36
(1,984)	1:60:C:LEU:H	1:80:C:GLN:H	2	0.36	0.12	0.36
(1,124)	1:44:A:LEU:HD21	1:133:A:PHE:HE1	2	0.34	0.15	0.34
(1,124)	1:44:A:LEU:HD21	1:133:A:PHE:HE2	2	0.34	0.15	0.34
(1,124)	1:44:A:LEU:HD22	1:133:A:PHE:HE1	2	0.34	0.15	0.34
(1,124)	1:44:A:LEU:HD22	1:133:A:PHE:HE2	2	0.34	0.15	0.34
(1,124)	1:44:A:LEU:HD23	1:133:A:PHE:HE1	2	0.34	0.15	0.34
(1,124)	1:44:A:LEU:HD23	1:133:A:PHE:HE2	2	0.34	0.15	0.34
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD11	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD12	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD13	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD11	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD12	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD13	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD11	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD12	2	0.34	0.04	0.34
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD13	2	0.34	0.04	0.34
(1,479)	1:39:B:GLU:H	1:67:B:SER:H	2	0.32	0.02	0.32
(1,19)	1:14:A:GLN:H	1:84:A:PHE:H	2	0.3	0.18	0.3
(1,184)	1:60:A:LEU:HD11	1:61:A:ARG:H	2	0.28	0.08	0.28
(1,184)	1:60:A:LEU:HD12	1:61:A:ARG:H	2	0.28	0.08	0.28
(1,184)	1:60:A:LEU:HD13	1:61:A:ARG:H	2	0.28	0.08	0.28
(1,382)	1:136:A:LEU:H	1:138:A:MET:H	2	0.28	0.01	0.28
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD11	2	0.26	0.06	0.26
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD12	2	0.26	0.06	0.26
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD13	2	0.26	0.06	0.26
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD11	2	0.26	0.06	0.26
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD12	2	0.26	0.06	0.26
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD13	2	0.26	0.06	0.26
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB1	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB2	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB3	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB1	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB2	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB3	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB1	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB2	2	0.24	0.02	0.24
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB3	2	0.24	0.02	0.24
(1,416)	1:14:B:GLN:H	1:84:B:PHE:HD1	2	0.24	0.04	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,416)	1:14:B:GLN:H	1:84:B:PHE:HD2	2	0.24	0.04	0.24
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG21	2	0.24	0.06	0.24
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG22	2	0.24	0.06	0.24
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG23	2	0.24	0.06	0.24
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG21	2	0.24	0.06	0.24
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG22	2	0.24	0.06	0.24
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG23	2	0.24	0.06	0.24
(1,560)	1:57:B:GLU:H	1:58:B:VAL:H	2	0.24	0.0	0.24
(1,1308)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	2	0.24	0.12	0.24
(1,1308)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	2	0.24	0.12	0.24
(1,1308)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	2	0.24	0.12	0.24
(1,1308)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	2	0.24	0.12	0.24
(1,1308)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	2	0.24	0.12	0.24
(1,1308)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	2	0.24	0.12	0.24
(1,329)	1:112:A:GLU:H	1:109:C:TYR:HE1	2	0.22	0.08	0.22
(1,329)	1:112:A:GLU:H	1:109:C:TYR:HE2	2	0.22	0.08	0.22
(1,1185)	1:136:C:LEU:H	1:138:C:MET:H	2	0.22	0.09	0.22
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG11	2	0.22	0.02	0.22
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG12	2	0.22	0.02	0.22
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG13	2	0.22	0.02	0.22
(1,1317)	1:47:D:ALA:H	1:61:D:ARG:H	2	0.22	0.04	0.22
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG11	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG12	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG13	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG11	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG12	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG13	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG11	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG12	2	0.21	0.06	0.21
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG13	2	0.21	0.06	0.21
(1,623)	1:68:B:LEU:H	1:72:B:THR:H	2	0.2	0.0	0.2
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG21	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG22	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG23	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG21	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG22	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG23	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG21	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG22	2	0.2	0.03	0.2
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG23	2	0.2	0.03	0.2
(1,927)	1:47:C:ALA:H	1:60:C:LEU:H	2	0.2	0.04	0.2
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD21	2	0.18	0.01	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD22	2	0.18	0.01	0.18
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD23	2	0.18	0.01	0.18
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD11	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD12	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD13	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD11	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD12	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD13	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD11	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD12	2	0.18	0.05	0.18
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD13	2	0.18	0.05	0.18
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG11	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG12	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG13	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG21	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG22	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG23	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG11	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG12	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG13	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG21	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG22	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG23	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG11	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG12	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG13	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG21	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG22	2	0.18	0.01	0.18
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG23	2	0.18	0.01	0.18
(1,212)	1:66:A:ALA:H	1:74:A:PHE:HE1	2	0.18	0.06	0.18
(1,212)	1:66:A:ALA:H	1:74:A:PHE:HE2	2	0.18	0.06	0.18
(1,1325)	1:49:D:SER:H	1:57:D:GLU:H	2	0.18	0.02	0.18
(1,192)	1:62:A:VAL:HG11	1:63:A:THR:H	2	0.17	0.03	0.17
(1,192)	1:62:A:VAL:HG12	1:63:A:THR:H	2	0.17	0.03	0.17
(1,192)	1:62:A:VAL:HG13	1:63:A:THR:H	2	0.17	0.03	0.17
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD21	2	0.17	0.05	0.17
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD22	2	0.17	0.05	0.17
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD23	2	0.17	0.05	0.17
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD21	2	0.17	0.05	0.17
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD22	2	0.17	0.05	0.17
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD23	2	0.17	0.05	0.17
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD21	2	0.17	0.05	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD22	2	0.17	0.05	0.17
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD23	2	0.17	0.05	0.17
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE1	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE2	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE3	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE1	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE2	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE3	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE1	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE2	2	0.17	0.01	0.17
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE3	2	0.17	0.01	0.17
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG21	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG22	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG23	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG21	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG22	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG23	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG21	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG22	2	0.16	0.02	0.16
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG23	2	0.16	0.02	0.16
(1,944)	1:51:C:LEU:H	1:56:C:TYR:H	2	0.16	0.06	0.16
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE1	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE2	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE3	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE1	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE2	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE3	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE1	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE2	2	0.16	0.04	0.16
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE3	2	0.16	0.04	0.16
(1,1029)	1:68:C:LEU:H	1:71:C:GLU:H	2	0.16	0.05	0.16
(1,1488)	1:98:D:LEU:H	1:100:D:ALA:H	2	0.16	0.0	0.16
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE1	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE2	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE3	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE1	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE2	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE3	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE1	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE2	2	0.16	0.01	0.16
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE3	2	0.16	0.01	0.16
(1,1543)	1:127:D:ASN:H	1:128:D:LEU:H	2	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	2	0.15	0.02	0.15
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	2	0.15	0.02	0.15
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG21	2	0.14	0.03	0.14
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG22	2	0.14	0.03	0.14
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG23	2	0.14	0.03	0.14
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG21	2	0.14	0.03	0.14
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG22	2	0.14	0.03	0.14
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG23	2	0.14	0.03	0.14
(1,69)	1:28:A:ALA:HB1	1:17:B:TYR:HE1	2	0.14	0.0	0.14
(1,69)	1:28:A:ALA:HB1	1:17:B:TYR:HE2	2	0.14	0.0	0.14
(1,69)	1:28:A:ALA:HB2	1:17:B:TYR:HE1	2	0.14	0.0	0.14
(1,69)	1:28:A:ALA:HB2	1:17:B:TYR:HE2	2	0.14	0.0	0.14
(1,69)	1:28:A:ALA:HB3	1:17:B:TYR:HE1	2	0.14	0.0	0.14
(1,69)	1:28:A:ALA:HB3	1:17:B:TYR:HE2	2	0.14	0.0	0.14
(1,757)	1:127:B:ASN:H	1:128:B:LEU:H	2	0.14	0.04	0.14
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD11	2	0.14	0.02	0.14
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD12	2	0.14	0.02	0.14
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD13	2	0.14	0.02	0.14
(1,1681)	1:131:D:VAL:HG11	2:462:H:TYR:HD1	2	0.14	0.02	0.14
(1,1681)	1:131:D:VAL:HG11	2:462:H:TYR:HD2	2	0.14	0.02	0.14
(1,1681)	1:131:D:VAL:HG12	2:462:H:TYR:HD1	2	0.14	0.02	0.14
(1,1681)	1:131:D:VAL:HG12	2:462:H:TYR:HD2	2	0.14	0.02	0.14
(1,1681)	1:131:D:VAL:HG13	2:462:H:TYR:HD1	2	0.14	0.02	0.14
(1,1681)	1:131:D:VAL:HG13	2:462:H:TYR:HD2	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD11	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD12	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD13	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD21	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD22	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD23	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD11	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD12	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD13	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD21	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD22	2	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD23	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD11	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD12	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD13	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD21	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD22	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD23	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD11	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD12	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD13	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD21	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD22	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD23	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD11	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD12	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD13	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD21	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD22	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD23	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD11	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD12	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD13	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD21	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD22	2	0.14	0.02	0.14
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD23	2	0.14	0.02	0.14
(1,50)	1:22:A:SER:H	1:79:A:GLN:H	2	0.13	0.0	0.13
(1,841)	1:22:C:SER:H	1:78:C:VAL:H	2	0.13	0.01	0.13
(1,1109)	1:99:C:GLY:H	1:100:C:ALA:H	2	0.12	0.02	0.12
(1,1485)	1:97:D:CYS:H	1:100:D:ALA:H	2	0.12	0.02	0.12
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD11	2	0.12	0.01	0.12
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD12	2	0.12	0.01	0.12
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD13	2	0.12	0.01	0.12
(1,449)	1:28:B:ALA:H	1:31:B:VAL:H	2	0.12	0.0	0.12
(1,621)	1:68:B:LEU:H	1:69:B:GLY:H	2	0.12	0.0	0.12
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD11	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD12	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD13	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD21	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD22	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD23	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD11	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD12	2	0.12	0.01	0.12

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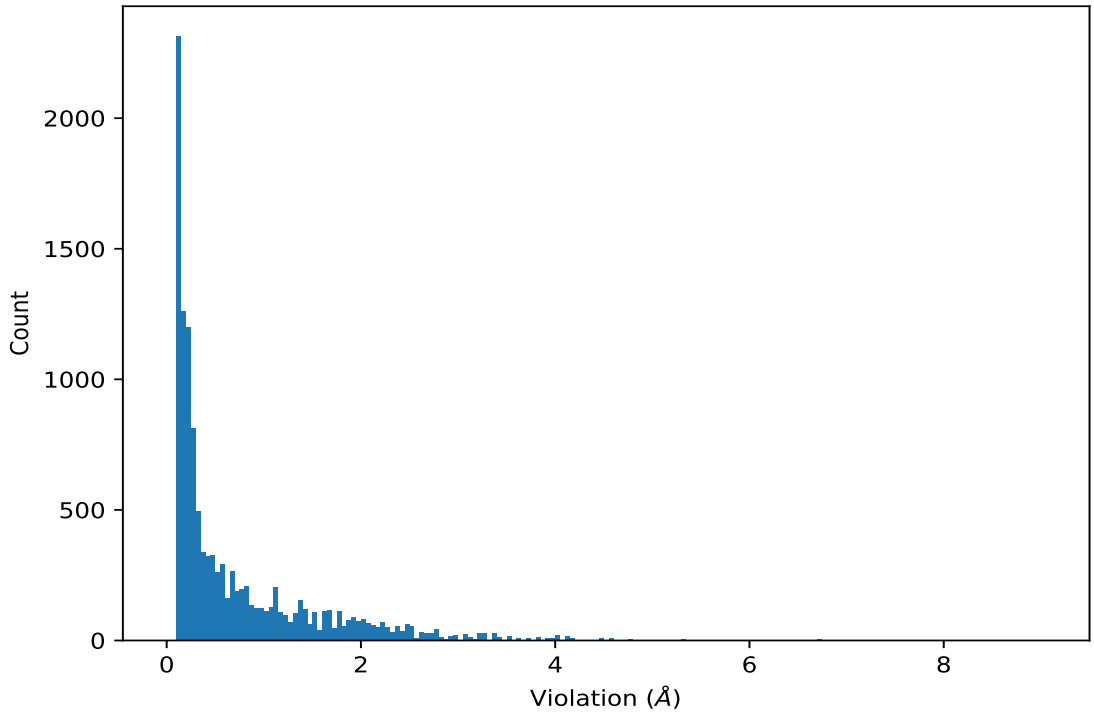
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD13	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD21	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD22	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD23	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD11	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD12	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD13	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD21	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD22	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD23	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD11	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD12	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD13	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD21	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD22	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD23	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD11	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD12	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD13	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD21	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD22	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD23	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD11	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD12	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD13	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD21	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD22	2	0.12	0.01	0.12
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD23	2	0.12	0.01	0.12
(1,1505)	1:110:D:ALA:H	1:111:D:ARG:H	2	0.12	0.02	0.12
(1,972)	1:58:C:VAL:H	1:59:C:VAL:H	2	0.12	0.0	0.12
(1,43)	1:21:A:ILE:H	1:22:A:SER:H	2	0.11	0.01	0.11
(1,720)	1:110:B:ALA:H	1:112:B:GLU:H	2	0.11	0.01	0.11
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD11	2	0.11	0.01	0.11
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD12	2	0.11	0.01	0.11
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD13	2	0.11	0.01	0.11
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD11	2	0.11	0.01	0.11
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD12	2	0.11	0.01	0.11
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD13	2	0.11	0.01	0.11
(1,226)	1:68:A:LEU:H	1:73:A:ALA:H	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	19	9.03
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	19	9.03
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE1	19	6.73
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE2	19	6.73
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE1	19	6.73
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE2	19	6.73
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE1	19	6.73
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE2	19	6.73
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	19	5.35
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	19	5.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	19	5.35
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	19	5.35
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	19	5.35
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	19	5.35
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	18	4.82
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	18	4.82
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	18	4.82
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	16	4.77
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	16	4.77
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	16	4.77
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	13	4.76
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	13	4.76
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	13	4.76
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	10	4.66
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	10	4.66
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	10	4.66
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	4	4.58
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	4	4.58
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	4	4.58
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	4	4.58
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	4	4.58
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	4	4.58
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	4	4.58
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	4	4.58
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	4	4.58
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	6	4.45
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	6	4.45
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	6	4.45
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	6	4.45
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	6	4.45
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	6	4.45
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	6	4.45
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	6	4.45
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	6	4.45
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	12	4.41
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	12	4.41
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	2	4.31
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	5	4.22
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	5	4.22
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	5	4.22
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	16	4.18
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	16	4.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	16	4.18
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	16	4.18
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	16	4.18
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	16	4.18
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	16	4.18
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	16	4.18
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	16	4.18
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	1	4.17
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	7	4.13
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	7	4.13
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	7	4.13
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	7	4.13
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	7	4.13
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	7	4.13
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	7	4.13
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	7	4.13
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	7	4.13
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	7	4.11
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	7	4.11
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	7	4.11
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	7	4.11
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	7	4.11
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	7	4.11
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	7	4.11
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	7	4.11
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	7	4.11
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	13	4.02
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	13	4.02
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	13	4.02
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	13	4.02
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	13	4.02
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	13	4.02
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	13	4.02
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	13	4.02
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	13	4.02
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	16	4.01
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	16	4.01
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	16	4.01
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	16	4.01
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	16	4.01
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	16	4.01
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	16	4.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	16	4.01
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	16	4.01
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	11	4.0
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	11	4.0
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	16	3.95
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	16	3.95
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	13	3.95
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	13	3.95
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	13	3.95
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	13	3.95
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	13	3.95
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	13	3.95
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	13	3.95
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	13	3.95
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	13	3.95
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	12	3.92
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	12	3.92
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	12	3.92
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	12	3.92
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	12	3.92
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	12	3.92
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	12	3.92
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	12	3.92
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	12	3.92
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	9	3.82
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	9	3.82
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	9	3.82
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	9	3.82
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	9	3.82
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	9	3.82
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	9	3.82
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	9	3.82
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	9	3.82
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	17	3.81
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	17	3.81
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	17	3.81
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	17	3.81
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	17	3.81
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	17	3.81
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	12	3.71
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	12	3.71
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	12	3.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	12	3.71
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	12	3.71
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	12	3.71
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	12	3.71
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	12	3.71
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	12	3.71
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	3	3.69
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	3	3.69
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	3	3.69
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	19	3.61
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	19	3.61
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	19	3.61
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	19	3.61
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	19	3.61
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	19	3.61
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	19	3.61
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	19	3.61
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	19	3.61
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	8	3.54
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	8	3.54
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	8	3.54
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	8	3.54
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	8	3.54
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	8	3.54
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	8	3.54
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	8	3.54
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	8	3.54
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	18	3.51
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	18	3.51
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	18	3.51
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	18	3.51
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	18	3.51
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	18	3.51
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	18	3.51
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	18	3.51
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	18	3.51
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	20	3.46
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	20	3.46
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	16	3.43
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	16	3.43
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	16	3.43
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	16	3.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	16	3.43
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	16	3.43
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	16	3.43
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	16	3.43
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	16	3.43
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	7	3.41
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	7	3.41
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	7	3.41
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	17	3.38
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	17	3.38
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	17	3.38
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	17	3.38
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	17	3.38
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	17	3.38
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	17	3.38
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	17	3.38
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	17	3.38
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD21	9	3.37
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD22	9	3.37
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD23	9	3.37
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD21	9	3.37
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD22	9	3.37
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD23	9	3.37
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD21	9	3.37
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD22	9	3.37
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD23	9	3.37
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	9	3.37
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	9	3.37
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	9	3.37
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	9	3.37
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	9	3.37
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	9	3.37
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	9	3.37
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	9	3.37
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	9	3.37
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	2	3.3
(1,939)	1:50:C:GLN:H	1:56:C:TYR:HE1	1	3.3
(1,939)	1:50:C:GLN:H	1:56:C:TYR:HE2	1	3.3
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	10	3.29
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	10	3.29
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	10	3.29
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	10	3.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	10	3.29
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	10	3.29
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	10	3.29
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	10	3.29
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	10	3.29
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	3	3.28
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	3	3.28
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	3	3.28
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	3	3.28
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	3	3.28
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	3	3.28
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	3	3.28
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	3	3.28
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	3	3.28
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	11	3.25
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	11	3.25
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	11	3.25
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	11	3.25
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	11	3.25
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	11	3.25
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	11	3.25
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	11	3.25
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	11	3.25
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	13	3.24
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	13	3.24
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	13	3.24
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	2	3.22
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	2	3.22
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	2	3.22
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	4	3.21
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	4	3.21
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	4	3.21
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	4	3.21
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	4	3.21
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	4	3.21
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	4	3.21
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	4	3.21
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	4	3.21
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	6	3.21
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	6	3.21
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	6	3.21
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	6	3.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	6	3.21
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	6	3.21
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	6	3.21
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	6	3.21
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	6	3.21
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	16	3.21
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	16	3.21
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	16	3.21
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	13	3.18
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	13	3.18
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	13	3.18
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	13	3.18
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	13	3.18
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	13	3.18
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	9	3.15
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	9	3.15
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	9	3.15
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	9	3.15
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	9	3.15
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	9	3.15
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	9	3.15
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	9	3.15
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	9	3.15
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	19	3.14
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	19	3.14
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	19	3.14
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	19	3.14
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	19	3.14
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	19	3.14
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	9	3.09
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	9	3.09
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	9	3.09
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	9	3.09
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	9	3.09
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	9	3.09
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	9	3.09
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	9	3.09
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	9	3.09
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	1	3.07
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	1	3.07
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	1	3.07
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	10	3.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	10	3.06
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	10	3.06
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	10	3.06
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	10	3.06
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	10	3.06
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	10	3.06
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	10	3.06
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	10	3.06
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	13	3.06
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	13	3.06
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	12	2.99
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	12	2.99
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	12	2.99
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	12	2.99
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	12	2.99
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	12	2.99
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	1	2.99
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	7	2.96
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	7	2.96
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	7	2.96
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	7	2.96
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	7	2.96
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	7	2.96
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	4	2.96
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	4	2.96
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	17	2.95
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	17	2.95
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	17	2.95
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	17	2.95
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	17	2.95
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	17	2.95
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD21	3	2.91
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD22	3	2.91
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD23	3	2.91
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD21	3	2.91
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD22	3	2.91
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD23	3	2.91
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD21	3	2.91
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD22	3	2.91
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD23	3	2.91
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	9	2.91
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	9	2.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	9	2.91
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	9	2.91
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	9	2.91
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	9	2.91
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	9	2.91
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	9	2.91
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	9	2.91
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	15	2.89
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	15	2.89
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	15	2.89
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	16	2.88
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	16	2.88
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	16	2.88
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	15	2.84
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	15	2.84
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	15	2.84
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD21	16	2.82
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD22	16	2.82
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD23	16	2.82
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD21	16	2.82
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD22	16	2.82
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD23	16	2.82
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD21	16	2.82
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD22	16	2.82
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD23	16	2.82
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	13	2.82
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	13	2.82
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	13	2.82
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	12	2.8
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	12	2.8
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	12	2.8
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	12	2.8
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	12	2.8
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	12	2.8
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	12	2.8
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	12	2.8
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	12	2.8
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	8	2.8
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	8	2.8
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	8	2.8
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	9	2.79
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	9	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	9	2.79
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	4	2.78
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	4	2.78
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	4	2.78
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	4	2.78
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	4	2.78
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	4	2.78
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	7	2.78
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	7	2.78
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	7	2.78
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	6	2.77
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	6	2.77
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	6	2.77
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	6	2.77
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	6	2.77
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	6	2.77
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	6	2.77
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	6	2.77
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	6	2.77
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	5	2.76
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	5	2.76
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD21	2	2.75
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD22	2	2.75
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD23	2	2.75
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD21	2	2.75
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD22	2	2.75
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD23	2	2.75
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD21	2	2.75
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD22	2	2.75
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD23	2	2.75
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	3	2.74
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	3	2.74
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	3	2.74
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	13	2.74
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	13	2.74
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	13	2.74
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	5	2.73
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	5	2.73
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	5	2.73
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	17	2.7
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	17	2.7
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	17	2.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	17	2.7
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	17	2.7
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	17	2.7
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	17	2.7
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	17	2.7
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	17	2.7
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	14	2.7
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	14	2.7
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	14	2.7
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	14	2.7
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	14	2.7
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	14	2.7
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	14	2.7
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	14	2.7
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	14	2.7
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	20	2.7
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	20	2.7
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	20	2.7
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	15	2.69
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	15	2.69
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	15	2.69
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	15	2.69
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	15	2.69
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	15	2.69
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	15	2.69
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	15	2.69
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	15	2.69
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	1	2.68
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	1	2.68
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	1	2.68
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	10	2.67
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	10	2.67
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	10	2.67
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	10	2.67
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	10	2.67
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	10	2.67
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	10	2.67
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	10	2.67
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	10	2.67
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	16	2.67
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	16	2.67
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	16	2.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	16	2.67
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	16	2.67
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	16	2.67
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	16	2.67
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	16	2.67
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	16	2.67
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	7	2.65
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	7	2.65
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	7	2.65
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	7	2.65
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	7	2.65
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	7	2.65
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	7	2.65
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	7	2.65
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	7	2.65
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	17	2.63
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	17	2.63
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	17	2.63
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	17	2.63
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	17	2.63
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	17	2.63
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	17	2.63
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	17	2.63
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	17	2.63
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	11	2.63
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	11	2.63
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	11	2.63
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	11	2.63
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	11	2.63
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	11	2.63
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	11	2.63
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	11	2.63
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	11	2.63
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	12	2.62
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	12	2.62
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	12	2.62
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	9	2.62
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	9	2.62
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	9	2.62
(1,1278)	1:36:D:TRP:HZ3	1:37:D:GLN:H	15	2.6
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	14	2.58
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	14	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	16	2.57
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	16	2.57
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	16	2.57
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	16	2.57
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	16	2.57
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	16	2.57
(1,1278)	1:36:D:TRP:HZ3	1:37:D:GLN:H	12	2.55
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	18	2.54
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	18	2.54
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	18	2.54
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	18	2.54
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	18	2.54
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	18	2.54
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	18	2.54
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	18	2.54
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	18	2.54
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	17	2.54
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	17	2.54
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	10	2.54
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	10	2.54
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	10	2.54
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	5	2.54
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	5	2.54
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	5	2.54
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	5	2.54
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	5	2.54
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	5	2.54
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	5	2.54
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	5	2.54
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	5	2.54
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	8	2.54
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	8	2.54
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	8	2.54
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	1	2.54
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	1	2.54
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	1	2.54
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	15	2.52
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	8	2.52
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	8	2.52
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	8	2.52
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	13	2.51
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	13	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	13	2.51
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	16	2.51
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	16	2.51
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	16	2.51
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	10	2.51
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	10	2.51
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	10	2.51
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	1	2.51
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	1	2.51
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	1	2.51
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	17	2.5
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	17	2.5
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	17	2.5
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	9	2.5
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	9	2.5
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	9	2.5
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	12	2.5
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	12	2.5
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	12	2.5
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	13	2.49
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	13	2.49
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	13	2.49
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	13	2.49
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	13	2.49
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	13	2.49
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	13	2.49
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	13	2.49
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	13	2.49
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	13	2.49
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	13	2.49
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	13	2.49
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	13	2.49
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	13	2.49
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	13	2.49
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	13	2.49
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	13	2.49
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	13	2.49
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	16	2.49
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	16	2.49
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	16	2.49
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	17	2.49
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	17	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	17	2.49
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	17	2.49
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	17	2.49
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	17	2.49
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	17	2.49
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	17	2.49
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	17	2.49
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	10	2.49
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	10	2.49
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	10	2.49
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	16	2.48
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	16	2.48
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	16	2.48
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	16	2.48
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	16	2.48
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	16	2.48
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	16	2.48
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	16	2.48
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	16	2.48
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	13	2.48
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	13	2.48
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	13	2.48
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	13	2.48
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	13	2.48
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	13	2.48
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	13	2.48
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	13	2.48
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	13	2.48
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	5	2.48
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	7	2.48
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	7	2.48
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	7	2.48
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	11	2.46
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	11	2.46
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	11	2.46
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	11	2.46
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	11	2.46
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	11	2.46
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	11	2.46
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	11	2.46
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	11	2.46
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	7	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	7	2.44
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	7	2.44
(1,1549)	1:131:D:VAL:HG11	1:133:D:PHE:HE1	12	2.43
(1,1549)	1:131:D:VAL:HG11	1:133:D:PHE:HE2	12	2.43
(1,1549)	1:131:D:VAL:HG12	1:133:D:PHE:HE1	12	2.43
(1,1549)	1:131:D:VAL:HG12	1:133:D:PHE:HE2	12	2.43
(1,1549)	1:131:D:VAL:HG13	1:133:D:PHE:HE1	12	2.43
(1,1549)	1:131:D:VAL:HG13	1:133:D:PHE:HE2	12	2.43
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	1	2.42
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	1	2.42
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	1	2.42
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	12	2.42
(1,1191)	1:137:C:PHE:HD1	1:141:C:LEU:H	6	2.42
(1,1191)	1:137:C:PHE:HD2	1:141:C:LEU:H	6	2.42
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	1	2.42
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	1	2.42
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	1	2.42
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	10	2.41
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	10	2.41
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	10	2.41
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	10	2.41
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	10	2.41
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	10	2.41
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	19	2.41
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	19	2.41
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	19	2.41
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD11	16	2.41
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD12	16	2.41
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD13	16	2.41
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD11	16	2.41
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD12	16	2.41
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD13	16	2.41
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD11	16	2.41
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD12	16	2.41
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD13	16	2.41
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	17	2.4
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	17	2.4
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	17	2.4
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	13	2.39
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	13	2.39
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	13	2.39
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	17	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	17	2.39
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	17	2.39
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	17	2.39
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	17	2.39
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	17	2.39
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	17	2.39
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	17	2.39
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	17	2.39
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	14	2.38
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	14	2.38
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	14	2.38
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	2	2.38
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	2	2.38
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	2	2.38
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD11	1	2.37
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD12	1	2.37
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD13	1	2.37
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD11	1	2.37
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD12	1	2.37
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD13	1	2.37
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	4	2.36
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	4	2.36
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	4	2.36
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	4	2.36
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	4	2.36
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	4	2.36
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	18	2.36
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	18	2.36
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	18	2.36
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	18	2.36
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	18	2.36
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	18	2.36
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	18	2.36
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	18	2.36
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	18	2.36
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	11	2.36
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	11	2.36
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	11	2.36
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	11	2.36
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	11	2.36
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	11	2.36
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	11	2.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	11	2.36
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	11	2.36
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	20	2.36
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	20	2.36
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	20	2.36
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	15	2.34
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	15	2.34
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	15	2.34
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	15	2.34
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	15	2.34
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	15	2.34
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	15	2.34
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	15	2.34
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	15	2.34
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	16	2.34
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	16	2.34
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	16	2.34
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	15	2.33
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	5	2.33
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	5	2.33
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	5	2.33
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	5	2.33
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	5	2.33
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	5	2.33
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	5	2.33
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	5	2.33
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	5	2.33
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	9	2.33
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	9	2.33
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	17	2.31
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	17	2.31
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	17	2.31
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	17	2.31
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	17	2.31
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	17	2.31
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	10	2.31
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	10	2.31
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	10	2.31
(1,476)	1:36:B:TRP:HZ3	1:37:B:GLN:H	12	2.31
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	5	2.3
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	5	2.3
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	5	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	7	2.3
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	7	2.3
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	7	2.3
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	7	2.3
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	7	2.3
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	7	2.3
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	7	2.3
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	7	2.3
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	7	2.3
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	12	2.29
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	6	2.29
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	6	2.29
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	6	2.29
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	17	2.29
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	17	2.29
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	13	2.29
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	13	2.29
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	13	2.29
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	7	2.29
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	7	2.29
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	7	2.29
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	7	2.28
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	7	2.28
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	7	2.28
(1,476)	1:36:B:TRP:HZ3	1:37:B:GLN:H	11	2.28
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	8	2.27
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	8	2.27
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	8	2.27
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	8	2.27
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	8	2.27
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	8	2.27
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	7	2.26
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	7	2.26
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	7	2.26
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	12	2.26
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	12	2.26
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	12	2.26
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	13	2.26
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	10	2.26
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	10	2.26
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	10	2.26
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	3	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	3	2.25
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	3	2.25
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	4	2.25
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	4	2.25
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	19	2.25
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	19	2.25
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	19	2.25
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	17	2.24
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	17	2.24
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	17	2.24
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	20	2.24
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	20	2.24
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	20	2.24
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	20	2.24
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	20	2.24
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	20	2.24
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	20	2.24
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	20	2.24
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	20	2.24
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	13	2.24
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	13	2.24
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	18	2.22
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	18	2.22
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	18	2.22
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	16	2.22
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	16	2.22
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	16	2.22
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	16	2.22
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	16	2.22
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	16	2.22
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	16	2.22
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	16	2.22
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	16	2.22
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	5	2.22
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	5	2.22
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	5	2.22
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	18	2.21
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	18	2.21
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	18	2.21
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	18	2.21
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	18	2.21
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	18	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	18	2.21
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	18	2.21
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	18	2.21
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	2	2.21
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	2	2.21
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	2	2.21
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	11	2.21
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	11	2.21
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	11	2.21
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	11	2.21
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	11	2.21
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	11	2.21
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	11	2.21
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	11	2.21
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	11	2.21
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD21	17	2.2
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD22	17	2.2
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD23	17	2.2
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD21	17	2.2
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD22	17	2.2
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD23	17	2.2
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD21	17	2.2
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD22	17	2.2
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD23	17	2.2
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	7	2.2
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	7	2.2
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	7	2.2
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	20	2.2
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	20	2.2
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	20	2.2
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	17	2.2
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	17	2.2
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	17	2.2
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	7	2.2
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	7	2.2
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	7	2.2
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	9	2.19
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	9	2.19
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	9	2.19
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	11	2.19
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	11	2.19
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	19	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	19	2.19
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	19	2.19
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	5	2.19
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	5	2.19
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	5	2.19
(1,938)	1:50:C:GLN:H	1:56:C:TYR:HD1	1	2.18
(1,938)	1:50:C:GLN:H	1:56:C:TYR:HD2	1	2.18
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	18	2.18
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	18	2.18
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	18	2.18
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	18	2.18
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	18	2.18
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	18	2.18
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	18	2.18
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	18	2.18
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	18	2.18
(1,476)	1:36:B:TRP:HZ3	1:37:B:GLN:H	15	2.18
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	19	2.17
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	19	2.17
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	19	2.17
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	19	2.17
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	19	2.17
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	19	2.17
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	19	2.17
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	19	2.17
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	19	2.17
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	1	2.16
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	1	2.16
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	11	2.16
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	11	2.16
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	11	2.16
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	14	2.15
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	14	2.15
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	14	2.15
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	15	2.15
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	15	2.15
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	15	2.15
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	15	2.15
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	15	2.15
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	15	2.15
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	15	2.15
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	15	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	15	2.15
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	11	2.15
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	11	2.15
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	11	2.15
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	19	2.14
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	19	2.14
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	19	2.14
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	2	2.14
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	2	2.14
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	2	2.14
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	2	2.14
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	2	2.14
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	2	2.14
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	2	2.14
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	2	2.14
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	2	2.14
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	14	2.14
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	14	2.14
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	14	2.14
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	4	2.13
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	4	2.13
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	4	2.13
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	6	2.13
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	6	2.13
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	6	2.13
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	6	2.13
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	6	2.13
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	6	2.13
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	6	2.13
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	6	2.13
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	6	2.13
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	2	2.13
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	2	2.13
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	2	2.13
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	2	2.13
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	2	2.13
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	2	2.13
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	2	2.13
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	2	2.13
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	2	2.13
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	8	2.12
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	8	2.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	8	2.12
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	12	2.12
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	12	2.12
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	6	2.12
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	6	2.12
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	6	2.12
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	15	2.12
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	15	2.12
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	15	2.12
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	10	2.11
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	10	2.11
(1,476)	1:36:B:TRP:HZ3	1:37:B:GLN:H	16	2.11
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	16	2.1
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	16	2.1
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	16	2.1
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	16	2.1
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	16	2.1
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	16	2.1
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	16	2.1
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	16	2.1
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	16	2.1
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	9	2.09
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	9	2.09
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	9	2.09
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	9	2.09
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	9	2.09
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	9	2.09
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	9	2.09
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	9	2.09
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	9	2.09
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	17	2.09
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	17	2.09
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	17	2.09
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	17	2.09
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	17	2.09
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	17	2.09
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	17	2.09
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	17	2.09
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	17	2.09
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	10	2.08
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	10	2.08
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	10	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	10	2.08
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	10	2.08
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	10	2.08
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	18	2.08
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	18	2.08
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	18	2.08
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	18	2.08
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	18	2.08
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	18	2.08
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	13	2.08
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	13	2.08
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	13	2.08
(1,1278)	1:36:D:TRP:HZ3	1:37:D:GLN:H	1	2.08
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	12	2.08
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	4	2.08
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	4	2.08
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	4	2.08
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	10	2.07
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	10	2.07
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	10	2.07
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	17	2.07
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	17	2.07
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	17	2.07
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	11	2.07
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	9	2.06
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	9	2.06
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	9	2.06
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	9	2.06
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	9	2.06
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	9	2.06
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	19	2.06
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	19	2.06
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	19	2.06
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	19	2.06
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	19	2.06
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	19	2.06
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	19	2.06
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	19	2.06
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	19	2.06
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	12	2.06
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	2	2.06
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	2	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	17	2.06
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	17	2.06
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	17	2.06
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	15	2.05
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	15	2.05
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	15	2.05
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	15	2.05
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	15	2.05
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	15	2.05
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	15	2.05
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	15	2.05
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	15	2.05
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	5	2.05
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	5	2.05
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	5	2.05
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	4	2.04
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	4	2.04
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	4	2.04
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	12	2.04
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	12	2.04
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	12	2.04
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	3	2.04
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	3	2.04
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	3	2.04
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	3	2.04
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	3	2.04
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	3	2.04
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	3	2.04
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	3	2.04
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	3	2.04
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	8	2.04
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	8	2.04
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	8	2.04
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	8	2.04
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	8	2.04
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	8	2.04
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	8	2.04
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	8	2.04
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	8	2.04
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	4	2.04
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	4	2.04
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	4	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	9	2.03
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	9	2.03
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	9	2.03
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	9	2.03
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	9	2.03
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	9	2.03
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	9	2.03
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	9	2.03
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	9	2.03
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	7	2.02
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	7	2.02
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	7	2.02
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	13	2.02
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	13	2.02
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	13	2.02
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	13	2.02
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	13	2.02
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	13	2.02
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	13	2.02
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	13	2.02
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	13	2.02
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	12	2.02
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	12	2.02
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	12	2.02
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	9	2.02
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	9	2.02
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	9	2.02
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	4	2.01
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	4	2.01
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	4	2.01
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	4	2.01
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	4	2.01
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	4	2.01
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	4	2.01
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	4	2.01
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	4	2.01
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	3	2.01
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	3	2.01
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	3	2.01
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	3	2.01
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	3	2.01
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	17	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	17	2.01
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	17	2.01
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	16	1.99
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	16	1.99
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	16	1.99
(1,906)	1:42:C:LEU:HD21	1:128:C:LEU:HD11	16	1.99
(1,906)	1:42:C:LEU:HD21	1:128:C:LEU:HD12	16	1.99
(1,906)	1:42:C:LEU:HD21	1:128:C:LEU:HD13	16	1.99
(1,906)	1:42:C:LEU:HD22	1:128:C:LEU:HD11	16	1.99
(1,906)	1:42:C:LEU:HD22	1:128:C:LEU:HD12	16	1.99
(1,906)	1:42:C:LEU:HD22	1:128:C:LEU:HD13	16	1.99
(1,906)	1:42:C:LEU:HD23	1:128:C:LEU:HD11	16	1.99
(1,906)	1:42:C:LEU:HD23	1:128:C:LEU:HD12	16	1.99
(1,906)	1:42:C:LEU:HD23	1:128:C:LEU:HD13	16	1.99
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	4	1.99
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	4	1.99
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	4	1.99
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	2	1.99
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	2	1.99
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	2	1.99
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	2	1.99
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	2	1.99
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	2	1.99
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	2	1.99
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	2	1.99
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	2	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	10	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	10	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	10	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	10	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	10	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	10	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	10	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	10	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	10	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	18	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	18	1.99
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	18	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	18	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	18	1.99
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	18	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	18	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	18	1.99
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	18	1.99
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	6	1.98
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	6	1.98
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	6	1.98
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	18	1.98
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	18	1.98
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	18	1.98
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	20	1.97
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	20	1.97
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	20	1.97
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	7	1.97
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	7	1.97
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	7	1.97
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	15	1.97
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	17	1.96
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	17	1.96
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	17	1.96
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	17	1.96
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	17	1.96
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	17	1.96
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	3	1.96
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	3	1.96
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	3	1.96
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	3	1.96
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	3	1.96
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	3	1.96
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	3	1.96
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	3	1.96
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	3	1.96
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	13	1.96
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	13	1.96
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	13	1.96
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	2	1.95
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	2	1.95
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	2	1.95
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	2	1.95
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	2	1.95
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	2	1.95
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	2	1.95
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	2	1.95
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	2	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	19	1.95
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	19	1.95
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	19	1.95
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	19	1.95
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	19	1.95
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	19	1.95
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	19	1.95
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	19	1.95
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	19	1.95
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	1	1.94
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	1	1.94
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	1	1.94
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	18	1.94
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	18	1.94
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	18	1.94
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD11	5	1.94
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD12	5	1.94
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD13	5	1.94
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD11	5	1.94
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD12	5	1.94
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD13	5	1.94
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	5	1.94
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	5	1.94
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	5	1.94
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	5	1.94
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	5	1.94
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	5	1.94
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	5	1.94
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	5	1.94
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	5	1.94
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	15	1.93
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	15	1.93
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	15	1.93
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	5	1.93
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	5	1.93
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	5	1.93
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD21	13	1.93
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD22	13	1.93
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD23	13	1.93
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD21	13	1.93
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD22	13	1.93
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD23	13	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD21	13	1.93
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD22	13	1.93
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD23	13	1.93
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	17	1.92
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	17	1.92
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	17	1.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	17	1.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	17	1.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	17	1.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	17	1.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	17	1.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	17	1.92
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD21	2	1.92
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD22	2	1.92
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD23	2	1.92
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD21	2	1.92
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD22	2	1.92
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD23	2	1.92
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD21	2	1.92
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD22	2	1.92
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD23	2	1.92
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	1	1.92
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	1	1.92
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	18	1.92
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	18	1.92
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	18	1.92
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	1	1.91
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD21	2	1.91
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD22	2	1.91
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD23	2	1.91
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD21	2	1.91
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD22	2	1.91
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD23	2	1.91
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD21	2	1.91
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD22	2	1.91
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD23	2	1.91
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	5	1.91
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	5	1.91
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	5	1.91
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	19	1.9
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	19	1.9
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	19	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE1	2	1.9
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE2	2	1.9
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE3	2	1.9
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	20	1.9
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	20	1.9
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	20	1.9
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	20	1.9
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	20	1.9
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	20	1.9
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	20	1.9
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	20	1.9
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	20	1.9
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	3	1.9
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	3	1.9
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	3	1.9
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	3	1.9
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	3	1.9
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	3	1.9
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	3	1.9
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	3	1.9
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	3	1.9
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	16	1.9
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	10	1.89
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	10	1.89
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	10	1.89
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD21	9	1.89
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD22	9	1.89
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD23	9	1.89
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD21	9	1.89
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD22	9	1.89
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD23	9	1.89
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD21	9	1.89
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD22	9	1.89
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD23	9	1.89
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	6	1.88
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	6	1.88
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	6	1.88
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	1	1.88
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	1	1.88
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	1	1.88
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	16	1.88
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	16	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	16	1.88
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	10	1.87
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	10	1.87
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	10	1.87
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	10	1.87
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	10	1.87
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	10	1.87
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	7	1.87
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	7	1.87
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	7	1.87
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	7	1.87
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	7	1.87
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	7	1.87
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	7	1.87
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	7	1.87
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	7	1.87
(1,476)	1:36:B:TRP:HZ3	1:37:B:GLN:H	5	1.86
(1,476)	1:36:B:TRP:HZ3	1:37:B:GLN:H	9	1.86
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	13	1.85
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	13	1.85
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	13	1.85
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	13	1.85
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	13	1.85
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	13	1.85
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	13	1.85
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	13	1.85
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	13	1.85
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	15	1.85
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	15	1.85
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	15	1.85
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	8	1.85
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	8	1.85
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	8	1.85
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	7	1.84
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	7	1.84
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	7	1.84
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	7	1.84
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	7	1.84
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	7	1.84
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	20	1.84
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	20	1.84
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	20	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	15	1.84
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	15	1.84
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD21	9	1.83
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD22	9	1.83
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD23	9	1.83
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD21	9	1.83
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD22	9	1.83
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD23	9	1.83
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD21	9	1.83
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD22	9	1.83
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD23	9	1.83
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	16	1.82
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	16	1.82
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	16	1.82
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	16	1.82
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	16	1.82
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	16	1.82
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	16	1.82
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	16	1.82
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	16	1.82
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	11	1.81
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	11	1.81
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	11	1.81
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	8	1.81
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	8	1.81
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	8	1.81
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	2	1.8
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	2	1.8
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	2	1.8
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	2	1.8
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	2	1.8
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	2	1.8
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	2	1.8
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	2	1.8
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	2	1.8
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	10	1.8
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	10	1.8
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	10	1.8
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	16	1.8
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	16	1.8
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	16	1.8
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	17	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	17	1.8
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	17	1.8
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	5	1.8
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	5	1.8
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	5	1.8
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	19	1.79
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	19	1.79
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	19	1.79
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	19	1.79
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	19	1.79
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	19	1.79
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	19	1.79
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	19	1.79
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	19	1.79
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD11	19	1.79
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD12	19	1.79
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD13	19	1.79
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD11	19	1.79
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD12	19	1.79
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD13	19	1.79
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	5	1.79
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	5	1.79
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	5	1.79
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	5	1.79
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	5	1.79
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	5	1.79
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	5	1.79
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	5	1.79
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	5	1.79
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD21	6	1.79
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD22	6	1.79
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD23	6	1.79
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD21	6	1.79
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD22	6	1.79
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD23	6	1.79
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD21	6	1.79
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD22	6	1.79
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD23	6	1.79
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	9	1.79
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	9	1.79
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	10	1.78
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	10	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	10	1.78
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	10	1.78
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	10	1.78
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	10	1.78
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	10	1.78
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	10	1.78
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	10	1.78
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	17	1.78
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	17	1.78
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	17	1.78
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	20	1.78
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	3	1.78
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	3	1.78
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	3	1.78
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	1	1.77
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	1	1.77
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	1	1.77
(1,686)	1:94:B:MET:HE1	1:95:B:ALA:H	2	1.77
(1,686)	1:94:B:MET:HE2	1:95:B:ALA:H	2	1.77
(1,686)	1:94:B:MET:HE3	1:95:B:ALA:H	2	1.77
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	11	1.77
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	11	1.77
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	11	1.77
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	20	1.77
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	20	1.77
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	20	1.77
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG11	12	1.77
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG12	12	1.77
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG13	12	1.77
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG11	12	1.77
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG12	12	1.77
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG13	12	1.77
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG11	12	1.77
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG12	12	1.77
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG13	12	1.77
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	1	1.77
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	1	1.77
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	1	1.77
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	1	1.77
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	1	1.77
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	1	1.77
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	1	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	1	1.77
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	1	1.77
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	3	1.76
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	3	1.76
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	3	1.76
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	3	1.76
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	3	1.76
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	3	1.76
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	3	1.76
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	3	1.76
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	3	1.76
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	5	1.76
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	5	1.76
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	5	1.76
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	14	1.76
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	14	1.76
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	18	1.76
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	18	1.76
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	18	1.76
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	13	1.75
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	13	1.75
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	13	1.75
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	13	1.75
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	13	1.75
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	13	1.75
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	19	1.75
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	19	1.75
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	19	1.75
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	19	1.75
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	19	1.75
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	19	1.75
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	19	1.75
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	19	1.75
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	19	1.75
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	6	1.74
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	6	1.74
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	6	1.74
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	17	1.74
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	17	1.74
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	17	1.74
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG11	16	1.74
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG12	16	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG13	16	1.74
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG11	16	1.74
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG12	16	1.74
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG13	16	1.74
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG11	16	1.74
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG12	16	1.74
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG13	16	1.74
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	14	1.73
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	14	1.73
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	14	1.73
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	19	1.72
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	19	1.72
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	19	1.72
(1,1278)	1:36:D:TRP:HZ3	1:37:D:GLN:H	2	1.72
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	20	1.72
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	20	1.72
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	20	1.72
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	20	1.72
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	20	1.72
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	20	1.72
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	20	1.72
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	20	1.72
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	20	1.72
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	13	1.72
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	13	1.72
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	13	1.72
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	12	1.71
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	12	1.71
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	12	1.71
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD11	15	1.71
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD12	15	1.71
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD13	15	1.71
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD11	15	1.71
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD12	15	1.71
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD13	15	1.71
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD11	15	1.71
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD12	15	1.71
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD13	15	1.71
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	7	1.7
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	7	1.7
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	8	1.7
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	8	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	8	1.7
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	20	1.7
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	20	1.7
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	20	1.7
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	20	1.7
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	20	1.7
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	20	1.7
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	20	1.7
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	20	1.7
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	20	1.7
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	12	1.7
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	12	1.7
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	12	1.7
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	5	1.7
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	9	1.7
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	3	1.69
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	3	1.69
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	3	1.69
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	3	1.69
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	3	1.69
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	3	1.69
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	3	1.69
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	3	1.69
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	3	1.69
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	7	1.69
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	7	1.69
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	7	1.69
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	18	1.69
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	18	1.69
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	18	1.69
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	11	1.69
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	11	1.69
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	11	1.69
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	3	1.69
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	3	1.69
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	18	1.69
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	18	1.69
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	18	1.69
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	7	1.69
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	7	1.69
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	7	1.69
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	7	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	7	1.69
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	7	1.69
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	7	1.69
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	7	1.69
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	7	1.69
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	1	1.69
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	1	1.69
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	1	1.69
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	8	1.68
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	8	1.68
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	8	1.68
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	11	1.68
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	11	1.68
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	11	1.68
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	11	1.68
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	11	1.68
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	11	1.68
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	11	1.68
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	11	1.68
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	11	1.68
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	5	1.68
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	5	1.68
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	5	1.68
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	5	1.68
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	5	1.68
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	5	1.68
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	4	1.67
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	4	1.67
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	4	1.67
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	15	1.67
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	15	1.67
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	15	1.67
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	9	1.67
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	9	1.67
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	9	1.67
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	6	1.66
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	6	1.66
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	6	1.66
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	4	1.66
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	4	1.66
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	4	1.66
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	16	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	16	1.66
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	16	1.66
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	16	1.66
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	16	1.66
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	16	1.66
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	16	1.66
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	16	1.66
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	16	1.66
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	16	1.66
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	16	1.66
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	16	1.66
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	20	1.66
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	20	1.66
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	20	1.66
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	20	1.66
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	20	1.66
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	20	1.66
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	19	1.66
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	19	1.66
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	19	1.66
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	19	1.66
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	19	1.66
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	19	1.66
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	19	1.66
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	19	1.66
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	19	1.66
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	11	1.66
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	11	1.66
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	11	1.66
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	18	1.65
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	18	1.65
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	18	1.65
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	18	1.65
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	18	1.65
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	18	1.65
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	18	1.65
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	18	1.65
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	18	1.65
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	5	1.65
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	5	1.65
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	5	1.65
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	4	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	4	1.65
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	4	1.65
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	12	1.65
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	14	1.65
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	14	1.65
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	14	1.65
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	14	1.65
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	14	1.65
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	14	1.65
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	14	1.65
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	14	1.65
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	14	1.65
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB1	11	1.65
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB2	11	1.65
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB3	11	1.65
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB1	11	1.65
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB2	11	1.65
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB3	11	1.65
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB1	11	1.65
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB2	11	1.65
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB3	11	1.65
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	18	1.64
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	18	1.64
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	18	1.64
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	18	1.64
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	18	1.64
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	18	1.64
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	18	1.64
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	18	1.64
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	18	1.64
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	2	1.64
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	2	1.64
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	2	1.64
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	20	1.64
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	20	1.64
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	20	1.64
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	15	1.63
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	15	1.63
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	15	1.63
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	9	1.63
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	9	1.63
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	9	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	9	1.63
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	9	1.63
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	9	1.63
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	9	1.63
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	9	1.63
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	9	1.63
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	2	1.62
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	18	1.62
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	18	1.62
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	18	1.62
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	18	1.62
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	18	1.62
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	18	1.62
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	18	1.62
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	18	1.62
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	18	1.62
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	13	1.62
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	13	1.62
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	13	1.62
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	13	1.62
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	13	1.62
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	13	1.62
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	13	1.62
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	13	1.62
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	13	1.62
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	17	1.61
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	17	1.61
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	17	1.61
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	8	1.61
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	8	1.61
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	8	1.61
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	8	1.61
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	8	1.61
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	8	1.61
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	8	1.61
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	8	1.61
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	8	1.61
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD11	3	1.6
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD12	3	1.6
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD13	3	1.6
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD11	3	1.6
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD12	3	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD13	3	1.6
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD11	3	1.6
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD12	3	1.6
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD13	3	1.6
(1,1192)	1:137:C:PHE:HE1	1:141:C:LEU:H	6	1.6
(1,1192)	1:137:C:PHE:HE2	1:141:C:LEU:H	6	1.6
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD11	16	1.6
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD12	16	1.6
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD13	16	1.6
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD11	16	1.6
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD12	16	1.6
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD13	16	1.6
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD11	16	1.6
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD12	16	1.6
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD13	16	1.6
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	11	1.6
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	11	1.6
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE1	4	1.59
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE2	4	1.59
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE3	4	1.59
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	9	1.58
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	9	1.58
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	9	1.58
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	9	1.58
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	9	1.58
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	9	1.58
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	9	1.58
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	9	1.58
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	9	1.58
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	20	1.57
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	20	1.57
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	20	1.57
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	2	1.56
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	2	1.56
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	2	1.56
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	2	1.55
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	2	1.55
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	2	1.55
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	2	1.55
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	2	1.55
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	2	1.55
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	2	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	2	1.55
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	2	1.55
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	19	1.55
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	19	1.55
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	19	1.55
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	19	1.55
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	19	1.55
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	19	1.55
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	19	1.55
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	19	1.55
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	19	1.55
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	19	1.55
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	19	1.55
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	19	1.55
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	18	1.54
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	18	1.54
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	18	1.54
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	12	1.54
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	12	1.54
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	12	1.54
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	12	1.54
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	12	1.54
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	12	1.54
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	12	1.54
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	12	1.54
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	12	1.54
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	20	1.53
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	20	1.53
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	20	1.53
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	20	1.53
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	20	1.53
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	20	1.53
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	16	1.53
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	16	1.53
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	16	1.53
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	16	1.53
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	16	1.53
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	16	1.53
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	16	1.53
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	16	1.53
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	16	1.53
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	2	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	2	1.52
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	2	1.52
(1,1549)	1:131:D:VAL:HG11	1:133:D:PHE:HE1	11	1.52
(1,1549)	1:131:D:VAL:HG11	1:133:D:PHE:HE2	11	1.52
(1,1549)	1:131:D:VAL:HG12	1:133:D:PHE:HE1	11	1.52
(1,1549)	1:131:D:VAL:HG12	1:133:D:PHE:HE2	11	1.52
(1,1549)	1:131:D:VAL:HG13	1:133:D:PHE:HE1	11	1.52
(1,1549)	1:131:D:VAL:HG13	1:133:D:PHE:HE2	11	1.52
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	12	1.52
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	12	1.52
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	12	1.52
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	12	1.52
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	12	1.52
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	12	1.52
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	12	1.52
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	12	1.52
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	12	1.52
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	9	1.52
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	9	1.52
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	9	1.52
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	15	1.52
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	15	1.52
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	15	1.52
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	15	1.52
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	15	1.52
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	15	1.52
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	15	1.52
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	15	1.52
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	15	1.52
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	5	1.52
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	5	1.52
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	5	1.52
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	10	1.52
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	10	1.52
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	10	1.52
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	10	1.52
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	10	1.52
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	10	1.52
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	10	1.52
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	10	1.52
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	10	1.52
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	18	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	18	1.51
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	18	1.51
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	5	1.51
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	5	1.51
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	5	1.51
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	5	1.51
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	5	1.51
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	5	1.51
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	10	1.51
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	10	1.51
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	10	1.51
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	10	1.51
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	10	1.51
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	10	1.51
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	10	1.51
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	10	1.51
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	10	1.51
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	3	1.5
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	3	1.5
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	3	1.5
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	10	1.5
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	10	1.5
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	10	1.5
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	10	1.5
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	10	1.5
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	10	1.5
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	10	1.5
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	10	1.5
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	10	1.5
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	2	1.5
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	2	1.5
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	2	1.5
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	10	1.5
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	10	1.5
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	10	1.5
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	10	1.5
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	10	1.5
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	10	1.5
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	2	1.49
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	2	1.49
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	2	1.49
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	2	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	2	1.49
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	2	1.49
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	2	1.49
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	2	1.49
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	2	1.49
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	15	1.49
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	15	1.49
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	15	1.49
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	15	1.49
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	15	1.49
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	15	1.49
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	15	1.49
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	15	1.49
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	15	1.49
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	16	1.48
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	16	1.48
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	16	1.48
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	3	1.47
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	3	1.47
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	3	1.47
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	9	1.47
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	9	1.47
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	9	1.47
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	9	1.47
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	9	1.47
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	9	1.47
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	6	1.47
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	6	1.47
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	6	1.47
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	6	1.47
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	6	1.47
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	6	1.47
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	7	1.47
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	7	1.47
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	7	1.47
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	9	1.47
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	12	1.46
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	12	1.46
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	12	1.46
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	12	1.46
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	12	1.46
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	12	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	12	1.46
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	12	1.46
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	12	1.46
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	6	1.46
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	6	1.46
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	6	1.46
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	13	1.46
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	13	1.46
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	13	1.46
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	10	1.46
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	10	1.46
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	10	1.46
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	9	1.46
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	9	1.46
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	9	1.46
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	13	1.46
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	13	1.46
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	13	1.46
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	6	1.45
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	6	1.45
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	6	1.45
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	6	1.45
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	6	1.45
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	6	1.45
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	6	1.45
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	6	1.45
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	6	1.45
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	6	1.45
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	6	1.45
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	5	1.45
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	5	1.45
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	5	1.45
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	11	1.44
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	11	1.44
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	11	1.44
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	8	1.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	3	1.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	3	1.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	3	1.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	3	1.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	3	1.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	3	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	6	1.44
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	6	1.44
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	6	1.44
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	4	1.44
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	4	1.44
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	4	1.44
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	4	1.44
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	4	1.44
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	4	1.44
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	4	1.44
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	4	1.44
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	4	1.44
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	15	1.44
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	15	1.44
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	15	1.44
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	15	1.44
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	15	1.44
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	15	1.44
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	15	1.44
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	15	1.44
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	15	1.44
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	7	1.43
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	7	1.43
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	7	1.43
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	9	1.43
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	9	1.43
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	9	1.43
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	9	1.43
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	9	1.43
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	9	1.43
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	9	1.43
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	9	1.43
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	9	1.43
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	8	1.43
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	8	1.43
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	8	1.43
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	18	1.43
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	18	1.43
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	18	1.43
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	9	1.43
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	9	1.43
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	9	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	9	1.43
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	9	1.43
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	9	1.43
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	9	1.43
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	9	1.43
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	9	1.43
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	8	1.43
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	8	1.43
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	8	1.43
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	5	1.42
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	5	1.42
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	5	1.42
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	5	1.42
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	5	1.42
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	5	1.42
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	5	1.42
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	5	1.42
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	5	1.42
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	20	1.42
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	20	1.42
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	20	1.42
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	7	1.42
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	7	1.42
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	7	1.42
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	7	1.42
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	7	1.42
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	7	1.42
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	2	1.42
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	2	1.42
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	2	1.42
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	20	1.41
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	20	1.41
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	20	1.41
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	20	1.41
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	20	1.41
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	20	1.41
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	20	1.41
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	20	1.41
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	20	1.41
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD11	13	1.41
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD12	13	1.41
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD13	13	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD11	13	1.41
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD12	13	1.41
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD13	13	1.41
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	6	1.41
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	6	1.41
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	6	1.41
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	6	1.41
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	6	1.41
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	6	1.41
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	6	1.41
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	6	1.41
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	6	1.41
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	4	1.4
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	4	1.4
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	4	1.4
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	4	1.4
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	4	1.4
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	4	1.4
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	4	1.4
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	4	1.4
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	4	1.4
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	2	1.4
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	2	1.4
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	2	1.4
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	2	1.4
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	2	1.4
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	2	1.4
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	4	1.4
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	4	1.4
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	4	1.4
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	4	1.4
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	4	1.4
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	4	1.4
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	4	1.4
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	4	1.4
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	4	1.4
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	10	1.4
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	10	1.4
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	10	1.4
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	9	1.39
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	9	1.39
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	9	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	18	1.39
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	18	1.39
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	18	1.39
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	13	1.39
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	13	1.39
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	13	1.39
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	13	1.39
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	13	1.39
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	13	1.39
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	13	1.39
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	13	1.39
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	13	1.39
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG21	5	1.39
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG22	5	1.39
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG23	5	1.39
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG21	5	1.39
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG22	5	1.39
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG23	5	1.39
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG21	5	1.39
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG22	5	1.39
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG23	5	1.39
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	14	1.39
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	14	1.39
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	3	1.38
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	3	1.38
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	3	1.38
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	17	1.38
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	17	1.38
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	17	1.38
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	10	1.38
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	10	1.38
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	10	1.38
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	15	1.38
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	17	1.38
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	17	1.38
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	10	1.37
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	10	1.37
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	10	1.37
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	11	1.37
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	11	1.37
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	11	1.37
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	11	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	11	1.37
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	11	1.37
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	11	1.37
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	11	1.37
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	11	1.37
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	10	1.37
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	10	1.37
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	10	1.37
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	10	1.37
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	10	1.37
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	10	1.37
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	10	1.37
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	10	1.37
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	10	1.37
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	10	1.37
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	11	1.37
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	11	1.37
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	11	1.37
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	4	1.37
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	4	1.37
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	4	1.37
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	4	1.37
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	4	1.37
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	4	1.37
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	4	1.37
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	4	1.37
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	4	1.37
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	4	1.36
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	4	1.36
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	4	1.36
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	10	1.36
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	10	1.36
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	10	1.36
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	14	1.36
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	14	1.36
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	14	1.36
(1,1198)	1:140:C:TYR:HE1	1:141:C:LEU:H	16	1.36
(1,1198)	1:140:C:TYR:HE2	1:141:C:LEU:H	16	1.36
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	7	1.36
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	18	1.36
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	18	1.36
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	18	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	12	1.36
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	13	1.35
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	13	1.35
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	13	1.35
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	13	1.35
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	13	1.35
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	13	1.35
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	13	1.35
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	13	1.35
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	13	1.35
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	4	1.35
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	4	1.35
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	4	1.35
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	4	1.35
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	4	1.35
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	4	1.35
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	6	1.35
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	6	1.35
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	6	1.35
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	6	1.35
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	6	1.35
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	6	1.35
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	6	1.35
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	6	1.35
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	6	1.35
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	20	1.35
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	20	1.35
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	20	1.35
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB1	3	1.35
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB2	3	1.35
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB3	3	1.35
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB1	3	1.35
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB2	3	1.35
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB3	3	1.35
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB1	3	1.35
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB2	3	1.35
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB3	3	1.35
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG21	13	1.35
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG22	13	1.35
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG23	13	1.35
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	15	1.34
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	15	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	15	1.34
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	3	1.34
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	1	1.34
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	1	1.34
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	3	1.34
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	3	1.34
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	3	1.34
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	3	1.34
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	3	1.34
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	3	1.34
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	3	1.34
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	3	1.34
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	3	1.34
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	8	1.33
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	8	1.33
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	8	1.33
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	8	1.33
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	8	1.33
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	8	1.33
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	8	1.33
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	8	1.33
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	8	1.33
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	4	1.33
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	4	1.33
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	4	1.33
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	4	1.33
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	4	1.33
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	4	1.33
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	4	1.33
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	4	1.33
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	4	1.33
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD11	3	1.32
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD12	3	1.32
(1,1554)	1:133:D:PHE:H	1:136:D:LEU:HD13	3	1.32
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	9	1.32
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	9	1.32
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	9	1.32
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	16	1.32
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	16	1.32
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	16	1.32
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	16	1.32
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	16	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	16	1.32
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	18	1.32
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	18	1.32
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	18	1.32
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	18	1.32
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	18	1.32
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	18	1.32
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	17	1.31
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	17	1.31
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	17	1.31
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	17	1.31
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	17	1.31
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	17	1.31
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	17	1.31
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	17	1.31
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	17	1.31
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	7	1.31
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	7	1.31
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	7	1.31
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG11	6	1.31
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG12	6	1.31
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG13	6	1.31
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG11	6	1.31
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG12	6	1.31
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG13	6	1.31
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG11	6	1.31
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG12	6	1.31
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG13	6	1.31
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	14	1.3
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	14	1.3
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	14	1.3
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	20	1.3
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	20	1.3
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	20	1.3
(1,945)	1:51:C:LEU:H	1:56:C:TYR:HD1	1	1.3
(1,945)	1:51:C:LEU:H	1:56:C:TYR:HD2	1	1.3
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	1	1.3
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	1	1.3
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	1	1.3
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	1	1.3
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	1	1.3
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	1	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	1	1.3
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	1	1.3
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	1	1.3
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	4	1.3
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	4	1.3
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	4	1.3
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	4	1.3
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	4	1.3
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	4	1.3
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	4	1.3
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	4	1.3
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	4	1.3
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	15	1.3
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	15	1.3
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	15	1.3
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	2	1.3
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE1	8	1.3
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE2	8	1.3
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE3	8	1.3
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	14	1.29
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	14	1.29
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	14	1.29
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	14	1.29
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	14	1.29
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	14	1.29
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	14	1.29
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	14	1.29
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	14	1.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	2	1.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	2	1.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	2	1.29
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	19	1.29
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	19	1.29
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	19	1.29
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	15	1.28
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	15	1.28
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	15	1.28
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	15	1.28
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	15	1.28
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	15	1.28
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	15	1.28
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	15	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	15	1.28
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	17	1.28
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	17	1.28
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	17	1.28
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	17	1.28
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	17	1.28
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	17	1.28
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	17	1.28
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	17	1.28
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	17	1.28
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	11	1.27
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	11	1.27
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	11	1.27
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD11	13	1.27
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD12	13	1.27
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD13	13	1.27
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD11	13	1.27
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD12	13	1.27
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD13	13	1.27
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD11	13	1.27
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD12	13	1.27
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD13	13	1.27
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	9	1.27
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	9	1.27
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	9	1.27
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD11	7	1.26
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD12	7	1.26
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD13	7	1.26
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD11	7	1.26
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD12	7	1.26
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD13	7	1.26
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	10	1.26
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	10	1.26
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	10	1.26
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	17	1.26
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	17	1.26
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	17	1.26
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB1	8	1.26
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB2	8	1.26
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB3	8	1.26
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB1	8	1.26
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB2	8	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB3	8	1.26
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB1	8	1.26
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB2	8	1.26
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB3	8	1.26
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	19	1.25
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	18	1.24
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	18	1.24
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	18	1.24
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	18	1.24
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	18	1.24
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	18	1.24
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	18	1.24
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	18	1.24
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	18	1.24
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	20	1.24
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	20	1.24
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	20	1.24
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	20	1.24
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	20	1.24
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	20	1.24
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	20	1.24
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	20	1.24
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	20	1.24
(1,1197)	1:140:C:TYR:HD1	1:141:C:LEU:H	16	1.24
(1,1197)	1:140:C:TYR:HD2	1:141:C:LEU:H	16	1.24
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG21	16	1.24
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG22	16	1.24
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG23	16	1.24
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG21	16	1.24
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG22	16	1.24
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG23	16	1.24
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG21	16	1.24
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG22	16	1.24
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG23	16	1.24
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	1	1.24
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	1	1.24
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	1	1.24
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	14	1.23
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	14	1.23
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	14	1.23
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD11	13	1.23
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD12	13	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD13	13	1.23
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD11	13	1.23
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD12	13	1.23
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD13	13	1.23
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD11	13	1.23
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD12	13	1.23
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD13	13	1.23
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD21	6	1.23
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD22	6	1.23
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD23	6	1.23
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD21	6	1.23
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD22	6	1.23
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD23	6	1.23
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD21	6	1.23
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD22	6	1.23
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD23	6	1.23
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	11	1.23
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	11	1.23
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	11	1.23
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	1	1.23
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	8	1.23
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	8	1.23
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	8	1.23
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	16	1.23
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	16	1.23
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	16	1.23
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	16	1.23
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	16	1.23
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	16	1.23
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	11	1.23
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	11	1.23
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	11	1.23
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	11	1.23
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	11	1.23
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	11	1.23
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	11	1.23
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	11	1.23
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	11	1.23
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	2	1.23
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	2	1.23
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	2	1.23
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	16	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	16	1.22
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	16	1.22
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	13	1.22
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	13	1.22
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	13	1.22
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	7	1.22
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	7	1.22
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	7	1.22
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	11	1.22
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	11	1.22
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	11	1.22
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	7	1.21
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	7	1.21
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	7	1.21
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	19	1.21
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	19	1.21
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	19	1.21
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	6	1.21
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	6	1.21
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	10	1.2
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	10	1.2
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	10	1.2
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	10	1.2
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	10	1.2
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	10	1.2
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	10	1.2
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	10	1.2
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	10	1.2
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	2	1.2
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	2	1.2
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	2	1.2
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	2	1.2
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	2	1.2
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	2	1.2
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	2	1.2
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	2	1.2
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	2	1.2
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	20	1.2
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	12	1.2
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	12	1.2
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	12	1.2
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	7	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	7	1.19
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	7	1.19
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	7	1.19
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	7	1.19
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	7	1.19
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	20	1.18
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	20	1.18
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	20	1.18
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	20	1.18
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	20	1.18
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	20	1.18
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	20	1.18
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	20	1.18
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	20	1.18
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	15	1.18
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	15	1.18
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	19	1.18
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	19	1.18
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	19	1.18
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	19	1.18
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	19	1.18
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	19	1.18
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	19	1.18
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	19	1.18
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	19	1.18
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	19	1.18
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	19	1.18
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	19	1.18
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	8	1.17
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	8	1.17
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	8	1.17
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	8	1.17
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	8	1.17
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	8	1.17
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	14	1.17
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	14	1.17
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	14	1.17
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	14	1.17
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	14	1.17
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	14	1.17
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	14	1.17
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	14	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	14	1.17
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	13	1.17
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	13	1.17
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	13	1.17
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	13	1.17
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	13	1.17
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	13	1.17
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	13	1.17
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	13	1.17
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	13	1.17
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	3	1.17
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	3	1.17
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	3	1.17
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	6	1.17
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	6	1.17
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	6	1.17
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	9	1.17
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	9	1.17
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	9	1.17
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	14	1.16
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	14	1.16
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	14	1.16
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	14	1.16
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	14	1.16
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	14	1.16
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	14	1.16
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	14	1.16
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	14	1.16
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	3	1.16
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	3	1.16
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	3	1.16
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	20	1.16
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	20	1.16
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	20	1.16
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD11	6	1.16
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD12	6	1.16
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD13	6	1.16
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD11	6	1.16
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD12	6	1.16
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD13	6	1.16
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD11	6	1.16
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD12	6	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD13	6	1.16
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	20	1.15
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	20	1.15
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	20	1.15
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	20	1.15
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	20	1.15
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	20	1.15
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	20	1.15
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	20	1.15
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	20	1.15
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	10	1.15
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	10	1.15
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	10	1.15
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	14	1.15
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	14	1.15
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	14	1.15
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	8	1.15
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	8	1.15
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	8	1.15
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	8	1.15
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	8	1.15
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	8	1.15
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	8	1.15
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	8	1.15
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	8	1.15
(1,367)	1:131:A:VAL:HG11	1:133:A:PHE:H	13	1.15
(1,367)	1:131:A:VAL:HG12	1:133:A:PHE:H	13	1.15
(1,367)	1:131:A:VAL:HG13	1:133:A:PHE:H	13	1.15
(1,118)	1:44:A:LEU:HD11	1:45:A:ASP:H	3	1.15
(1,118)	1:44:A:LEU:HD12	1:45:A:ASP:H	3	1.15
(1,118)	1:44:A:LEU:HD13	1:45:A:ASP:H	3	1.15
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	13	1.14
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	13	1.14
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	13	1.14
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	13	1.14
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	13	1.14
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	13	1.14
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	13	1.14
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	13	1.14
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	13	1.14
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	15	1.14
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	15	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	15	1.14
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG11	17	1.14
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG12	17	1.14
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG13	17	1.14
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG11	17	1.14
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG12	17	1.14
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG13	17	1.14
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG11	17	1.14
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG12	17	1.14
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG13	17	1.14
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD21	3	1.14
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD22	3	1.14
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD23	3	1.14
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD21	3	1.14
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD22	3	1.14
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD23	3	1.14
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD21	3	1.14
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD22	3	1.14
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD23	3	1.14
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD21	15	1.14
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD22	15	1.14
(1,905)	1:42:C:LEU:HD21	1:44:C:LEU:HD23	15	1.14
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD21	15	1.14
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD22	15	1.14
(1,905)	1:42:C:LEU:HD22	1:44:C:LEU:HD23	15	1.14
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD21	15	1.14
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD22	15	1.14
(1,905)	1:42:C:LEU:HD23	1:44:C:LEU:HD23	15	1.14
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG11	12	1.14
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG12	12	1.14
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG13	12	1.14
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG11	12	1.14
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG12	12	1.14
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG13	12	1.14
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG11	12	1.14
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG12	12	1.14
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG13	12	1.14
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	10	1.14
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	10	1.14
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	10	1.14
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	10	1.14
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	10	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	10	1.14
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	10	1.14
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	10	1.14
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	10	1.14
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG21	13	1.14
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG22	13	1.14
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG23	13	1.14
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG21	13	1.14
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG22	13	1.14
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG23	13	1.14
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG21	13	1.14
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG22	13	1.14
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG23	13	1.14
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	20	1.14
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	20	1.14
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	20	1.14
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	14	1.13
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	14	1.13
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	14	1.13
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD11	8	1.13
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD12	8	1.13
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD13	8	1.13
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD11	8	1.13
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD12	8	1.13
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD13	8	1.13
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	4	1.13
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	4	1.13
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	4	1.13
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	4	1.13
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	4	1.13
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	4	1.13
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	4	1.13
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	4	1.13
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	4	1.13
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	9	1.13
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	9	1.13
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	9	1.13
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	9	1.13
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	9	1.13
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	9	1.13
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	9	1.13
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	9	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	9	1.13
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	7	1.12
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	7	1.12
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	7	1.12
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	7	1.12
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	7	1.12
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	7	1.12
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	15	1.12
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	15	1.12
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	15	1.12
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	11	1.12
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	11	1.12
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	11	1.12
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	11	1.12
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	11	1.12
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	11	1.12
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	11	1.12
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	11	1.12
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	11	1.12
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	20	1.12
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	20	1.12
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	20	1.12
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	20	1.12
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	20	1.12
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	20	1.12
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	20	1.12
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	20	1.12
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	20	1.12
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	5	1.12
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	5	1.12
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	5	1.12
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	5	1.12
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	5	1.12
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	5	1.12
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	5	1.12
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	5	1.12
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	5	1.12
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	2	1.11
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	2	1.11
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	2	1.11
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	2	1.11
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	2	1.11
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	2	1.11
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	2	1.11
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	2	1.11
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	14	1.11
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	14	1.11
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	14	1.11
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	14	1.11
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	14	1.11
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	14	1.11
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	14	1.11
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	14	1.11
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	14	1.11
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	8	1.11
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	8	1.11
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	8	1.11
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	18	1.1
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	18	1.1
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	18	1.1
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	18	1.1
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	18	1.1
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	18	1.1
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	17	1.1
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	17	1.1
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	17	1.1
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD11	15	1.1
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD12	15	1.1
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD13	15	1.1
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD11	15	1.1
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD12	15	1.1
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD13	15	1.1
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	5	1.1
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	5	1.1
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	5	1.1
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	4	1.1
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	4	1.1
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	4	1.1
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	14	1.09
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	14	1.09
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	14	1.09
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	14	1.09
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	14	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	14	1.09
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	14	1.09
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	14	1.09
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	14	1.09
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	11	1.09
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	11	1.09
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	11	1.09
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	11	1.09
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	11	1.09
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	11	1.09
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	11	1.09
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	11	1.09
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	11	1.09
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	15	1.09
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	15	1.09
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	5	1.08
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	5	1.08
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	5	1.08
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	14	1.08
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	9	1.08
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	9	1.08
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	9	1.08
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	13	1.08
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	13	1.08
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	13	1.08
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	10	1.08
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	8	1.08
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	8	1.08
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	8	1.08
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	2	1.07
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	12	1.07
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	12	1.07
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	12	1.07
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	12	1.07
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	12	1.07
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	12	1.07
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	12	1.07
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	12	1.07
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	12	1.07
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	17	1.07
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	17	1.07
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	17	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	17	1.07
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	17	1.07
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	17	1.07
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG21	6	1.07
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG22	6	1.07
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG23	6	1.07
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	17	1.07
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	17	1.07
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	17	1.07
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	16	1.06
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	16	1.06
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	16	1.06
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	16	1.06
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	16	1.06
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	16	1.06
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	16	1.06
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	16	1.06
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	16	1.06
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	11	1.06
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	11	1.06
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	11	1.06
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	11	1.06
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	11	1.06
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	11	1.06
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	11	1.06
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	11	1.06
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	11	1.06
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	14	1.06
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	14	1.06
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	14	1.06
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	14	1.06
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	14	1.06
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	14	1.06
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	14	1.06
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	14	1.06
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	14	1.06
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	17	1.06
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	17	1.06
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	17	1.06
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	17	1.06
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	17	1.06
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	17	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	17	1.06
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	17	1.06
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	17	1.06
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	16	1.06
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	16	1.06
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	16	1.06
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	9	1.06
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	9	1.06
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	9	1.06
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	12	1.05
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	12	1.05
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	12	1.05
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	12	1.05
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	12	1.05
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	12	1.05
(1,1278)	1:36:D:TRP:HZ3	1:37:D:GLN:H	17	1.05
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE1	17	1.05
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE2	17	1.05
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE3	17	1.05
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	6	1.05
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	6	1.05
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	6	1.05
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	6	1.05
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	6	1.05
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	6	1.05
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	6	1.05
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	6	1.05
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	6	1.05
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	16	1.05
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	16	1.05
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	17	1.05
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	17	1.05
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	17	1.05
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	17	1.05
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	17	1.05
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	17	1.05
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	17	1.05
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	17	1.05
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	17	1.05
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	15	1.04
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	15	1.04
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	15	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	4	1.04
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD11	10	1.04
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD12	10	1.04
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD13	10	1.04
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD11	10	1.04
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD12	10	1.04
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD13	10	1.04
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	6	1.04
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	6	1.04
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	6	1.04
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	16	1.04
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	16	1.04
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	16	1.04
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	17	1.03
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	17	1.03
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	17	1.03
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	19	1.03
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	19	1.03
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	19	1.03
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	14	1.03
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	14	1.03
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	14	1.03
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	5	1.03
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	5	1.03
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	5	1.03
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	5	1.03
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	5	1.03
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	5	1.03
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	5	1.03
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	5	1.03
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	5	1.03
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	11	1.03
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	11	1.03
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	11	1.03
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	11	1.03
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	11	1.03
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	11	1.03
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	11	1.03
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	11	1.03
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	11	1.03
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	7	1.03
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	7	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	11	1.02
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	11	1.02
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	11	1.02
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	11	1.02
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	11	1.02
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	11	1.02
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	11	1.02
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	11	1.02
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	11	1.02
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	13	1.02
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	13	1.02
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	12	1.02
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	12	1.02
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	12	1.02
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	12	1.02
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	12	1.02
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	12	1.02
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	12	1.02
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	12	1.02
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	12	1.02
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	2	1.02
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	2	1.02
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	2	1.02
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	15	1.02
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	15	1.02
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	15	1.02
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	16	1.01
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	10	1.01
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	10	1.01
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	10	1.01
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	10	1.01
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	10	1.01
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	10	1.01
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	7	1.01
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	7	1.01
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	7	1.01
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	7	1.01
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	7	1.01
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	7	1.01
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	7	1.01
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	7	1.01
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	7	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	10	1.01
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	10	1.01
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	6	1.01
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	1	1.0
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	1	1.0
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	1	1.0
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	7	1.0
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	14	1.0
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	14	1.0
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	14	1.0
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	10	1.0
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	10	1.0
(1,686)	1:94:B:MET:HE1	1:95:B:ALA:H	7	1.0
(1,686)	1:94:B:MET:HE2	1:95:B:ALA:H	7	1.0
(1,686)	1:94:B:MET:HE3	1:95:B:ALA:H	7	1.0
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	9	1.0
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	9	1.0
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	9	1.0
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	9	1.0
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	9	1.0
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	9	1.0
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE1	8	1.0
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE2	8	1.0
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE3	8	1.0
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE1	8	1.0
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE2	8	1.0
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE3	8	1.0
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	14	0.99
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	14	0.99
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	14	0.99
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	14	0.99
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	14	0.99
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	14	0.99
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	14	0.99
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	14	0.99
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	14	0.99
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	10	0.99
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	10	0.99
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	10	0.99
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	10	0.99
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	10	0.99
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	10	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	14	0.99
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	14	0.99
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	14	0.99
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	14	0.99
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	14	0.99
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	14	0.99
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	14	0.99
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	14	0.99
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	14	0.99
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	15	0.99
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	15	0.99
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	15	0.99
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	7	0.99
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	7	0.99
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	7	0.99
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	7	0.99
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	7	0.99
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	7	0.99
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	7	0.99
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	7	0.99
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	7	0.99
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	1	0.99
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	1	0.99
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	1	0.99
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE1	17	0.99
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE2	17	0.99
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE3	17	0.99
(1,1196)	1:140:C:TYR:H	1:141:C:LEU:H	6	0.98
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	6	0.98
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	6	0.98
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	11	0.98
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	11	0.98
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	11	0.98
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	11	0.98
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	11	0.98
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	11	0.98
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	11	0.98
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	11	0.98
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	11	0.98
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	1	0.98
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	1	0.98
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	1	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	1	0.98
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	1	0.98
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	1	0.98
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	1	0.98
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	1	0.98
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	1	0.98
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	3	0.98
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	3	0.98
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	3	0.98
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	19	0.98
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	19	0.98
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	19	0.98
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	13	0.98
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	5	0.98
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	9	0.98
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG21	19	0.98
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG22	19	0.98
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG23	19	0.98
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE1	12	0.97
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE2	12	0.97
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD21	7	0.97
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD22	7	0.97
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD23	7	0.97
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD21	7	0.97
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD22	7	0.97
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD23	7	0.97
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD21	7	0.97
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD22	7	0.97
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD23	7	0.97
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	12	0.97
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	18	0.97
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	18	0.97
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	13	0.97
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG21	14	0.97
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG22	14	0.97
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG23	14	0.97
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG21	14	0.97
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG22	14	0.97
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG23	14	0.97
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG21	14	0.97
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG22	14	0.97
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG23	14	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	19	0.97
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	19	0.97
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	19	0.97
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	5	0.96
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	5	0.96
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	5	0.96
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	17	0.96
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG11	18	0.96
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG12	18	0.96
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG13	18	0.96
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG11	18	0.96
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG12	18	0.96
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG13	18	0.96
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG11	18	0.96
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG12	18	0.96
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG13	18	0.96
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	6	0.96
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	6	0.96
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	6	0.96
(1,367)	1:131:A:VAL:HG11	1:133:A:PHE:H	7	0.96
(1,367)	1:131:A:VAL:HG12	1:133:A:PHE:H	7	0.96
(1,367)	1:131:A:VAL:HG13	1:133:A:PHE:H	7	0.96
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	14	0.96
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	14	0.96
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	14	0.96
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	6	0.95
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	6	0.95
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	6	0.95
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	6	0.95
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	6	0.95
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	6	0.95
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	6	0.95
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	6	0.95
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	6	0.95
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	2	0.95
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	2	0.95
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	4	0.95
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	4	0.95
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	4	0.95
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	5	0.94
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	5	0.94
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	5	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE1	17	0.94
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE2	17	0.94
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE3	17	0.94
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE1	17	0.94
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE2	17	0.94
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE3	17	0.94
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	1	0.93
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	1	0.93
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	1	0.93
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	3	0.93
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	3	0.93
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	3	0.93
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	12	0.93
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	12	0.93
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	12	0.93
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	2	0.93
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	2	0.93
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	2	0.93
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE1	17	0.92
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE2	17	0.92
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	4	0.92
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	4	0.92
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	4	0.92
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	4	0.92
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	4	0.92
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	4	0.92
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	16	0.92
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	16	0.92
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	16	0.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	16	0.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	16	0.92
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	16	0.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	16	0.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	16	0.92
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	16	0.92
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	9	0.92
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	9	0.92
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	1	0.92
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	1	0.92
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	1	0.92
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	1	0.92
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	1	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	1	0.92
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	1	0.92
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	1	0.92
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	1	0.92
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	3	0.92
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	3	0.92
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	3	0.92
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	2	0.92
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	2	0.92
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	2	0.92
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	17	0.92
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	17	0.92
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	15	0.92
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	15	0.92
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	15	0.92
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	18	0.91
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	2	0.91
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD21	10	0.91
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD22	10	0.91
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD23	10	0.91
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD21	10	0.91
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD22	10	0.91
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD23	10	0.91
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD21	10	0.91
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD22	10	0.91
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD23	10	0.91
(1,686)	1:94:B:MET:HE1	1:95:B:ALA:H	15	0.91
(1,686)	1:94:B:MET:HE2	1:95:B:ALA:H	15	0.91
(1,686)	1:94:B:MET:HE3	1:95:B:ALA:H	15	0.91
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG21	19	0.91
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG22	19	0.91
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG23	19	0.91
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG21	19	0.91
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG22	19	0.91
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG23	19	0.91
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG21	19	0.91
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG22	19	0.91
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG23	19	0.91
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	3	0.91
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	3	0.91
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	3	0.91
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	3	0.91
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	3	0.91
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	3	0.91
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	3	0.91
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	3	0.91
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	13	0.91
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	13	0.91
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	13	0.91
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	5	0.91
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	5	0.91
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	5	0.91
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	8	0.91
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	8	0.91
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	8	0.91
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	4	0.9
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	4	0.9
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	11	0.9
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	4	0.9
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	4	0.9
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	4	0.9
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	11	0.9
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	11	0.9
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	11	0.9
(1,1546)	1:128:D:LEU:HD21	1:129:D:ALA:H	8	0.89
(1,1546)	1:128:D:LEU:HD22	1:129:D:ALA:H	8	0.89
(1,1546)	1:128:D:LEU:HD23	1:129:D:ALA:H	8	0.89
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	2	0.89
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	2	0.89
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	2	0.89
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	2	0.89
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	2	0.89
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	2	0.89
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	2	0.89
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	2	0.89
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	2	0.89
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	11	0.89
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	1	0.89
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG11	2	0.89
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG12	2	0.89
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG13	2	0.89
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG11	2	0.89
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG12	2	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG13	2	0.89
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG11	2	0.89
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG12	2	0.89
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG13	2	0.89
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD11	17	0.89
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD12	17	0.89
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD13	17	0.89
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD11	17	0.89
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD12	17	0.89
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD13	17	0.89
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	15	0.89
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	4	0.89
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	4	0.89
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	6	0.89
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	6	0.89
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	20	0.88
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	6	0.88
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	17	0.88
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	17	0.88
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	17	0.88
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	17	0.88
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	17	0.88
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	17	0.88
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	17	0.88
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	17	0.88
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	17	0.88
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD11	1	0.88
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD12	1	0.88
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD13	1	0.88
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD11	1	0.88
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD12	1	0.88
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD13	1	0.88
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	4	0.88
(1,349)	1:118:A:VAL:HG11	1:123:A:PHE:HD1	14	0.88
(1,349)	1:118:A:VAL:HG11	1:123:A:PHE:HD2	14	0.88
(1,349)	1:118:A:VAL:HG12	1:123:A:PHE:HD1	14	0.88
(1,349)	1:118:A:VAL:HG12	1:123:A:PHE:HD2	14	0.88
(1,349)	1:118:A:VAL:HG13	1:123:A:PHE:HD1	14	0.88
(1,349)	1:118:A:VAL:HG13	1:123:A:PHE:HD2	14	0.88
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD21	17	0.88
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD22	17	0.88
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD23	17	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD21	17	0.88
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD22	17	0.88
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD23	17	0.88
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD21	17	0.88
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD22	17	0.88
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD23	17	0.88
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG21	19	0.88
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG22	19	0.88
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG23	19	0.88
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG21	19	0.88
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG22	19	0.88
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG23	19	0.88
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG21	19	0.88
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG22	19	0.88
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG23	19	0.88
(1,164)	1:56:A:TYR:H	1:86:A:ILE:H	9	0.88
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG11	15	0.88
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG12	15	0.88
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG13	15	0.88
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	15	0.88
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	15	0.88
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	15	0.88
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	13	0.87
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	13	0.87
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	13	0.87
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	13	0.87
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	13	0.87
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	13	0.87
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	9	0.87
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	20	0.87
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	20	0.87
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	11	0.87
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	11	0.87
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	11	0.87
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	11	0.87
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	11	0.87
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	11	0.87
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	6	0.87
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	6	0.87
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	6	0.87
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	6	0.87
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	6	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	6	0.87
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	6	0.87
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	6	0.87
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	6	0.87
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	19	0.87
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	19	0.87
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	19	0.87
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	7	0.87
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	7	0.87
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	7	0.87
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	7	0.86
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	7	0.86
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	7	0.86
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	17	0.86
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	17	0.86
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	17	0.86
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	17	0.86
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	17	0.86
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	17	0.86
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	17	0.86
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	17	0.86
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	17	0.86
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	16	0.86
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	13	0.86
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG21	18	0.86
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG22	18	0.86
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG23	18	0.86
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	15	0.86
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	10	0.86
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	10	0.86
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	10	0.86
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	13	0.85
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	4	0.85
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	7	0.85
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	7	0.85
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	7	0.85
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	7	0.85
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	7	0.85
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	7	0.85
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	7	0.85
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	7	0.85
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	7	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	20	0.85
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	20	0.85
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	20	0.85
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	5	0.85
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	5	0.85
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	5	0.85
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	5	0.85
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	5	0.85
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	5	0.85
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	5	0.85
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	5	0.85
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	5	0.85
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	16	0.85
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	16	0.85
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	1	0.85
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	1	0.85
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	1	0.85
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	6	0.84
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	6	0.84
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	6	0.84
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	6	0.84
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	6	0.84
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	6	0.84
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	9	0.84
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	15	0.84
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	15	0.84
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	15	0.84
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	7	0.84
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	7	0.84
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	7	0.84
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	7	0.84
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	7	0.84
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	7	0.84
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	3	0.84
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	3	0.84
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	3	0.84
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	15	0.84
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	7	0.84
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	7	0.84
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	19	0.84
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	19	0.84
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	19	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	2	0.84
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	2	0.84
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	3	0.84
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	9	0.84
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	9	0.84
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	20	0.84
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	20	0.84
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	2	0.83
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	11	0.83
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	8	0.83
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	8	0.83
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	8	0.83
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	8	0.83
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	8	0.83
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	8	0.83
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	8	0.83
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	8	0.83
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	8	0.83
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	7	0.83
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	7	0.83
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	7	0.83
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD11	16	0.83
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD12	16	0.83
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD13	16	0.83
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD11	16	0.83
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD12	16	0.83
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD13	16	0.83
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	15	0.83
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	15	0.83
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	15	0.83
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	15	0.83
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	15	0.83
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	15	0.83
(1,369)	1:131:A:VAL:HG11	1:136:A:LEU:HD21	6	0.83
(1,369)	1:131:A:VAL:HG11	1:136:A:LEU:HD22	6	0.83
(1,369)	1:131:A:VAL:HG11	1:136:A:LEU:HD23	6	0.83
(1,369)	1:131:A:VAL:HG12	1:136:A:LEU:HD21	6	0.83
(1,369)	1:131:A:VAL:HG12	1:136:A:LEU:HD22	6	0.83
(1,369)	1:131:A:VAL:HG12	1:136:A:LEU:HD23	6	0.83
(1,369)	1:131:A:VAL:HG13	1:136:A:LEU:HD21	6	0.83
(1,369)	1:131:A:VAL:HG13	1:136:A:LEU:HD22	6	0.83
(1,369)	1:131:A:VAL:HG13	1:136:A:LEU:HD23	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	10	0.83
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	3	0.83
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	3	0.83
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	3	0.83
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	5	0.83
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	5	0.83
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	5	0.83
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	5	0.83
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	5	0.83
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	5	0.83
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	5	0.83
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	5	0.83
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	5	0.83
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	9	0.83
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	9	0.83
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	9	0.83
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	3	0.82
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	3	0.82
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	3	0.82
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	3	0.82
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	3	0.82
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	3	0.82
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	3	0.82
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	3	0.82
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	3	0.82
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	17	0.82
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE1	8	0.82
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE2	8	0.82
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE3	8	0.82
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD11	5	0.82
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD12	5	0.82
(1,85)	1:35:A:ASP:H	1:68:A:LEU:HD13	5	0.82
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	5	0.81
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	7	0.81
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	4	0.81
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	4	0.81
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	4	0.81
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	4	0.81
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	4	0.81
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	4	0.81
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	2	0.81
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	2	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	2	0.81
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	2	0.81
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	2	0.81
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	2	0.81
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	2	0.81
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	2	0.81
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	2	0.81
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	18	0.81
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	18	0.81
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	18	0.81
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	15	0.81
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	15	0.81
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	15	0.81
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	6	0.81
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	11	0.81
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	11	0.81
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	11	0.81
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	17	0.81
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	12	0.81
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	12	0.81
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	18	0.8
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	18	0.8
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	18	0.8
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	18	0.8
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	18	0.8
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	18	0.8
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE1	18	0.8
(1,1171)	1:131:C:VAL:HG11	1:133:C:PHE:HE2	18	0.8
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE1	18	0.8
(1,1171)	1:131:C:VAL:HG12	1:133:C:PHE:HE2	18	0.8
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE1	18	0.8
(1,1171)	1:131:C:VAL:HG13	1:133:C:PHE:HE2	18	0.8
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	8	0.8
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	8	0.8
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	8	0.8
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	8	0.8
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	8	0.8
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	8	0.8
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	8	0.8
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	8	0.8
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	8	0.8
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	6	0.8
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	6	0.8
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	6	0.8
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	6	0.8
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	6	0.8
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	6	0.8
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	6	0.8
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	6	0.8
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	8	0.8
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	8	0.8
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	8	0.8
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	8	0.8
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	8	0.8
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	8	0.8
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	8	0.8
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	8	0.8
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	8	0.8
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	17	0.8
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	17	0.8
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	17	0.8
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	17	0.8
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	17	0.8
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	17	0.8
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	17	0.8
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	17	0.8
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	17	0.8
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	3	0.8
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	3	0.8
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	3	0.8
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	7	0.79
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	7	0.79
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	7	0.79
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD21	10	0.79
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD22	10	0.79
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD23	10	0.79
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD21	10	0.79
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD22	10	0.79
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD23	10	0.79
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD21	10	0.79
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD22	10	0.79
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD23	10	0.79
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	3	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	3	0.79
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	3	0.79
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	3	0.79
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	3	0.79
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	3	0.79
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	11	0.79
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	11	0.79
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	11	0.79
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD11	18	0.79
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD12	18	0.79
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD13	18	0.79
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD11	18	0.79
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD12	18	0.79
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD13	18	0.79
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	8	0.79
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	8	0.79
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	20	0.79
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	20	0.79
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	20	0.79
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	20	0.79
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	20	0.79
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	20	0.79
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	1	0.79
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	1	0.79
(1,349)	1:118:A:VAL:HG11	1:123:A:PHE:HD1	7	0.79
(1,349)	1:118:A:VAL:HG11	1:123:A:PHE:HD2	7	0.79
(1,349)	1:118:A:VAL:HG12	1:123:A:PHE:HD1	7	0.79
(1,349)	1:118:A:VAL:HG12	1:123:A:PHE:HD2	7	0.79
(1,349)	1:118:A:VAL:HG13	1:123:A:PHE:HD1	7	0.79
(1,349)	1:118:A:VAL:HG13	1:123:A:PHE:HD2	7	0.79
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG21	20	0.79
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG22	20	0.79
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG23	20	0.79
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG21	20	0.79
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG22	20	0.79
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG23	20	0.79
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG21	20	0.79
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG22	20	0.79
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG23	20	0.79
(1,122)	1:44:A:LEU:HD21	1:45:A:ASP:H	3	0.79
(1,122)	1:44:A:LEU:HD22	1:45:A:ASP:H	3	0.79
(1,122)	1:44:A:LEU:HD23	1:45:A:ASP:H	3	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	12	0.78
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	12	0.78
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	12	0.78
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	12	0.78
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	12	0.78
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	12	0.78
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD21	18	0.78
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD22	18	0.78
(1,1299)	1:43:D:ASP:H	1:44:D:LEU:HD23	18	0.78
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	14	0.78
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	14	0.78
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	14	0.78
(1,888)	1:39:C:GLU:H	1:67:C:SER:H	12	0.78
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD21	7	0.78
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD22	7	0.78
(1,602)	1:64:B:VAL:HG21	1:126:B:LEU:HD23	7	0.78
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD21	7	0.78
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD22	7	0.78
(1,602)	1:64:B:VAL:HG22	1:126:B:LEU:HD23	7	0.78
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD21	7	0.78
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD22	7	0.78
(1,602)	1:64:B:VAL:HG23	1:126:B:LEU:HD23	7	0.78
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	9	0.78
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	9	0.78
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	9	0.78
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD1	18	0.77
(1,1170)	1:131:C:VAL:HG11	1:133:C:PHE:HD2	18	0.77
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD1	18	0.77
(1,1170)	1:131:C:VAL:HG12	1:133:C:PHE:HD2	18	0.77
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD1	18	0.77
(1,1170)	1:131:C:VAL:HG13	1:133:C:PHE:HD2	18	0.77
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	19	0.77
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	19	0.77
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	19	0.77
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	7	0.77
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	12	0.77
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	9	0.77
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	9	0.77
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	9	0.77
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	6	0.77
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	6	0.77
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	6	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	6	0.77
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	6	0.77
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	6	0.77
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	6	0.77
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	6	0.77
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	6	0.77
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	11	0.77
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	8	0.77
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	19	0.77
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	19	0.77
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	13	0.76
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	5	0.76
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	11	0.76
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	11	0.76
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	11	0.76
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	11	0.76
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	11	0.76
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	11	0.76
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	6	0.76
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	9	0.76
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	15	0.76
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	11	0.76
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	11	0.76
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	11	0.76
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	11	0.76
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	11	0.76
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	11	0.76
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	11	0.76
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	11	0.76
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	11	0.76
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	4	0.76
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	19	0.76
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	19	0.76
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	6	0.76
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD11	2	0.76
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD12	2	0.76
(1,496)	1:42:B:LEU:H	1:128:B:LEU:HD13	2	0.76
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	1	0.76
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	1	0.76
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	1	0.76
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	1	0.76
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	1	0.76
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	1	0.76
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	1	0.76
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	1	0.76
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	5	0.76
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	5	0.76
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	5	0.76
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	20	0.76
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	20	0.76
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	20	0.76
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	20	0.76
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	20	0.76
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	18	0.76
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	18	0.76
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	12	0.75
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	12	0.75
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	12	0.75
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	12	0.75
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	12	0.75
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	12	0.75
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	12	0.75
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	12	0.75
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	12	0.75
(1,1189)	1:137:C:PHE:H	1:140:C:TYR:H	6	0.75
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	9	0.75
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	9	0.75
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	9	0.75
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	17	0.75
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	19	0.75
(1,674)	1:90:B:GLU:H	1:94:B:MET:H	17	0.75
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	7	0.75
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	7	0.75
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	7	0.75
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	7	0.75
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	7	0.75
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	7	0.75
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	7	0.75
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	7	0.75
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	7	0.75
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	7	0.75
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	7	0.75
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	7	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	7	0.75
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	7	0.75
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	7	0.75
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	7	0.75
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	7	0.75
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	7	0.75
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	15	0.75
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	15	0.75
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	15	0.75
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	17	0.75
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	10	0.75
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	8	0.75
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD11	1	0.75
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD12	1	0.75
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD13	1	0.75
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	13	0.75
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	13	0.75
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	19	0.74
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	19	0.74
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	19	0.74
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	19	0.74
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	19	0.74
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	19	0.74
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	19	0.74
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	19	0.74
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	19	0.74
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	4	0.74
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	4	0.74
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	4	0.74
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	2	0.74
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	2	0.74
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	2	0.74
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	2	0.74
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	2	0.74
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	2	0.74
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	17	0.74
(1,1169)	1:131:C:VAL:HG11	1:133:C:PHE:H	4	0.74
(1,1169)	1:131:C:VAL:HG12	1:133:C:PHE:H	4	0.74
(1,1169)	1:131:C:VAL:HG13	1:133:C:PHE:H	4	0.74
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	16	0.74
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	14	0.74
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	19	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	19	0.74
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	19	0.74
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	19	0.74
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	19	0.74
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	19	0.74
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	19	0.74
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	19	0.74
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	19	0.74
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	18	0.74
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	7	0.74
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	7	0.74
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	7	0.74
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	7	0.74
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	7	0.74
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	7	0.74
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	7	0.74
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	7	0.74
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	7	0.74
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	13	0.74
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	13	0.74
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	13	0.74
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	13	0.74
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	13	0.74
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	13	0.74
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	5	0.74
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	5	0.74
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	5	0.74
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	5	0.74
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	5	0.74
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	5	0.74
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	5	0.74
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	5	0.74
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	5	0.74
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	12	0.74
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	12	0.74
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	12	0.74
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	12	0.74
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	12	0.74
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	12	0.74
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	12	0.74
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	12	0.74
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	12	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	3	0.74
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	3	0.74
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	12	0.74
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG21	15	0.74
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG22	15	0.74
(1,137)	1:49:A:SER:H	1:58:A:VAL:HG23	15	0.74
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG11	13	0.74
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG12	13	0.74
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG13	13	0.74
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	14	0.73
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	15	0.73
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD21	12	0.73
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD22	12	0.73
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD23	12	0.73
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD21	12	0.73
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD22	12	0.73
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD23	12	0.73
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD21	12	0.73
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD22	12	0.73
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD23	12	0.73
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD11	3	0.73
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD12	3	0.73
(1,968)	1:56:C:TYR:HD1	1:98:C:LEU:HD13	3	0.73
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD11	3	0.73
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD12	3	0.73
(1,968)	1:56:C:TYR:HD2	1:98:C:LEU:HD13	3	0.73
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	2	0.73
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD21	10	0.73
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD22	10	0.73
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD23	10	0.73
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD21	10	0.73
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD22	10	0.73
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD23	10	0.73
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD21	10	0.73
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD22	10	0.73
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD23	10	0.73
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	17	0.73
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	17	0.73
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	17	0.73
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	12	0.73
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	12	0.73
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	12	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	2	0.73
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	2	0.73
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	2	0.73
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	19	0.73
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	19	0.73
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	19	0.73
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	11	0.73
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	11	0.73
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	2	0.72
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	2	0.72
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	2	0.72
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	2	0.72
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	2	0.72
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	2	0.72
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	7	0.72
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	7	0.72
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	12	0.72
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	12	0.72
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	12	0.72
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	8	0.72
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	20	0.72
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	7	0.72
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	2	0.72
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	2	0.72
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	2	0.72
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	2	0.72
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	2	0.72
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	2	0.72
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	2	0.72
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	2	0.72
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	2	0.72
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	19	0.72
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	18	0.72
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	12	0.72
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	12	0.72
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	12	0.72
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	3	0.72
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	12	0.72
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	18	0.71
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	18	0.71
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	18	0.71
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	4	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	4	0.71
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	4	0.71
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	4	0.71
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	4	0.71
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	4	0.71
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	4	0.71
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	4	0.71
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	4	0.71
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	18	0.71
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	20	0.71
(1,888)	1:39:C:GLU:H	1:67:C:SER:H	18	0.71
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	20	0.71
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE1	14	0.71
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE2	14	0.71
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE3	14	0.71
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD11	6	0.71
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD12	6	0.71
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD13	6	0.71
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD11	6	0.71
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD12	6	0.71
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD13	6	0.71
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD11	6	0.71
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD12	6	0.71
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD13	6	0.71
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	3	0.71
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	3	0.71
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	3	0.71
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	3	0.71
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	3	0.71
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	3	0.71
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	3	0.71
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	3	0.71
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	3	0.71
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	16	0.71
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	5	0.71
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	1	0.71
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	10	0.71
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	10	0.71
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	2	0.7
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	2	0.7
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	2	0.7
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD21	19	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD22	19	0.7
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD23	19	0.7
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD21	19	0.7
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD22	19	0.7
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD23	19	0.7
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD21	19	0.7
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD22	19	0.7
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD23	19	0.7
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	11	0.7
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	20	0.7
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	18	0.7
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	18	0.7
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	2	0.7
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	2	0.7
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	2	0.7
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD11	9	0.7
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD12	9	0.7
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD13	9	0.7
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD11	9	0.7
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD12	9	0.7
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD13	9	0.7
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD11	9	0.7
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD12	9	0.7
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD13	9	0.7
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD21	9	0.7
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD22	9	0.7
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD23	9	0.7
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD21	9	0.7
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD22	9	0.7
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD23	9	0.7
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	19	0.7
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	19	0.7
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	19	0.7
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	19	0.7
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	19	0.7
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	19	0.7
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	19	0.7
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	19	0.7
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	19	0.7
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD11	7	0.7
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD12	7	0.7
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD13	7	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD11	7	0.7
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD12	7	0.7
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD13	7	0.7
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD11	7	0.7
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD12	7	0.7
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD13	7	0.7
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	6	0.7
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	4	0.7
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	10	0.7
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	3	0.7
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	3	0.7
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	14	0.69
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	14	0.69
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	14	0.69
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	14	0.69
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	14	0.69
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	14	0.69
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	1	0.69
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	16	0.69
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	16	0.69
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	14	0.69
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	11	0.69
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	11	0.69
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	12	0.69
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	12	0.69
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	12	0.69
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	12	0.69
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	12	0.69
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	12	0.69
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	12	0.69
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	12	0.69
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	12	0.69
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	13	0.69
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	13	0.69
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	13	0.69
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	13	0.69
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	13	0.69
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	13	0.69
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	13	0.69
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	13	0.69
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	13	0.69
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	10	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	10	0.69
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	10	0.69
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	19	0.69
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	19	0.69
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	19	0.69
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	1	0.69
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD21	20	0.69
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD22	20	0.69
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD23	20	0.69
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD21	20	0.69
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD22	20	0.69
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD23	20	0.69
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD21	20	0.69
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD22	20	0.69
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD23	20	0.69
(1,177)	1:59:A:VAL:HG11	1:81:A:GLY:H	8	0.69
(1,177)	1:59:A:VAL:HG12	1:81:A:GLY:H	8	0.69
(1,177)	1:59:A:VAL:HG13	1:81:A:GLY:H	8	0.69
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	3	0.69
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	3	0.69
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	7	0.68
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	7	0.68
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	7	0.68
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	7	0.68
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	7	0.68
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	7	0.68
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	12	0.68
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	12	0.68
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	12	0.68
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	3	0.68
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	20	0.68
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	13	0.68
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	13	0.68
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	13	0.68
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	3	0.68
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD1	12	0.68
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD2	12	0.68
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	13	0.68
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	13	0.68
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	13	0.68
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	12	0.68
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	19	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	9	0.68
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	13	0.68
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	8	0.68
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	8	0.68
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	8	0.68
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	8	0.68
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	8	0.68
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	8	0.68
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	8	0.68
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	8	0.68
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	8	0.68
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	16	0.68
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	16	0.68
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	16	0.68
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	12	0.67
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	12	0.67
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	12	0.67
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	12	0.67
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	12	0.67
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	12	0.67
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	4	0.67
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	18	0.67
(1,1169)	1:131:C:VAL:HG11	1:133:C:PHE:H	10	0.67
(1,1169)	1:131:C:VAL:HG12	1:133:C:PHE:H	10	0.67
(1,1169)	1:131:C:VAL:HG13	1:133:C:PHE:H	10	0.67
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	14	0.67
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	14	0.67
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	14	0.67
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	10	0.67
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	19	0.67
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	19	0.67
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	14	0.67
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	14	0.67
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD21	17	0.67
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD22	17	0.67
(1,761)	1:131:B:VAL:HG11	1:136:B:LEU:HD23	17	0.67
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD21	17	0.67
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD22	17	0.67
(1,761)	1:131:B:VAL:HG12	1:136:B:LEU:HD23	17	0.67
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD21	17	0.67
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD22	17	0.67
(1,761)	1:131:B:VAL:HG13	1:136:B:LEU:HD23	17	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	10	0.67
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	10	0.67
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	10	0.67
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	10	0.67
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	10	0.67
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	10	0.67
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	10	0.67
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	10	0.67
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	10	0.67
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	5	0.67
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	15	0.67
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	8	0.67
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	16	0.67
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	16	0.67
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	16	0.67
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	20	0.67
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	14	0.67
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	17	0.67
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	17	0.67
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	14	0.67
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	16	0.67
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	16	0.67
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	11	0.66
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	11	0.66
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	11	0.66
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	16	0.66
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	16	0.66
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	16	0.66
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	19	0.66
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	5	0.66
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	17	0.66
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	20	0.66
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	20	0.66
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	20	0.66
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	10	0.66
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	10	0.66
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	10	0.66
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	10	0.66
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	10	0.66
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	10	0.66
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	10	0.66
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	10	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	10	0.66
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	7	0.66
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	8	0.66
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	7	0.66
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	19	0.66
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	19	0.66
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	19	0.66
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	19	0.66
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	19	0.66
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	19	0.66
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	19	0.66
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	19	0.66
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	19	0.66
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	6	0.66
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	6	0.66
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	6	0.66
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	17	0.66
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	8	0.66
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	19	0.66
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	18	0.66
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	18	0.66
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	18	0.66
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	15	0.66
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	15	0.66
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	5	0.65
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	5	0.65
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	5	0.65
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	6	0.65
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	6	0.65
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	6	0.65
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	10	0.65
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	14	0.65
(1,555)	1:56:B:TYR:H	1:86:B:ILE:H	17	0.65
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	7	0.65
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	7	0.65
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	7	0.65
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	7	0.65
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	7	0.65
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	7	0.65
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	7	0.65
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	7	0.65
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	9	0.65
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	9	0.65
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	9	0.65
(1,348)	1:118:A:VAL:HG11	1:123:A:PHE:H	1	0.65
(1,348)	1:118:A:VAL:HG12	1:123:A:PHE:H	1	0.65
(1,348)	1:118:A:VAL:HG13	1:123:A:PHE:H	1	0.65
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	9	0.65
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	5	0.65
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	6	0.65
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	7	0.65
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	5	0.64
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	13	0.64
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	13	0.64
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	13	0.64
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	6	0.64
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	6	0.64
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	6	0.64
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	16	0.64
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	15	0.64
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	15	0.64
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	15	0.64
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	1	0.64
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	2	0.64
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	2	0.64
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	15	0.64
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	7	0.64
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	16	0.64
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD11	16	0.64
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD12	16	0.64
(1,599)	1:64:B:VAL:HG11	1:126:B:LEU:HD13	16	0.64
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD11	16	0.64
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD12	16	0.64
(1,599)	1:64:B:VAL:HG12	1:126:B:LEU:HD13	16	0.64
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD11	16	0.64
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD12	16	0.64
(1,599)	1:64:B:VAL:HG13	1:126:B:LEU:HD13	16	0.64
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	20	0.64
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	20	0.64
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	20	0.64
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	18	0.64
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	18	0.64
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	18	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	18	0.64
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	18	0.64
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	18	0.64
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	18	0.64
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	18	0.64
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	18	0.64
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	18	0.64
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	7	0.64
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	7	0.64
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	7	0.64
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	19	0.63
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	1	0.63
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	1	0.63
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	1	0.63
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	16	0.63
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	16	0.63
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	16	0.63
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	8	0.63
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	8	0.63
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	6	0.63
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	1	0.63
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	10	0.63
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	15	0.63
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	7	0.63
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	16	0.63
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD21	6	0.63
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD22	6	0.63
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD23	6	0.63
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD21	6	0.63
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD22	6	0.63
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD23	6	0.63
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	9	0.63
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	12	0.63
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	19	0.63
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	1	0.63
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD11	9	0.63
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD12	9	0.63
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD13	9	0.63
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	7	0.62
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	7	0.62
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	7	0.62
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	4	0.62
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	4	0.62
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	9	0.62
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	9	0.62
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD11	9	0.62
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD12	9	0.62
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD13	9	0.62
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD11	9	0.62
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD12	9	0.62
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD13	9	0.62
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD11	9	0.62
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD12	9	0.62
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD13	9	0.62
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG11	13	0.62
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG12	13	0.62
(1,902)	1:42:C:LEU:HD11	1:64:C:VAL:HG13	13	0.62
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG11	13	0.62
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG12	13	0.62
(1,902)	1:42:C:LEU:HD12	1:64:C:VAL:HG13	13	0.62
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG11	13	0.62
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG12	13	0.62
(1,902)	1:42:C:LEU:HD13	1:64:C:VAL:HG13	13	0.62
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	11	0.62
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	11	0.62
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	11	0.62
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	4	0.62
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	4	0.62
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE1	6	0.62
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE2	6	0.62
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE1	6	0.62
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE2	6	0.62
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE1	6	0.62
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE2	6	0.62
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	15	0.62
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	15	0.62
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	15	0.62
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	16	0.62
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	16	0.62
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	16	0.62
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	9	0.61
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	9	0.61
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	14	0.61
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	5	0.61
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	5	0.61
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	5	0.61
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	5	0.61
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	5	0.61
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	5	0.61
(1,1297)	1:42:D:LEU:HD21	1:129:D:ALA:H	7	0.61
(1,1297)	1:42:D:LEU:HD22	1:129:D:ALA:H	7	0.61
(1,1297)	1:42:D:LEU:HD23	1:129:D:ALA:H	7	0.61
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	10	0.61
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	10	0.61
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	19	0.61
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD11	7	0.61
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD12	7	0.61
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD13	7	0.61
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD11	7	0.61
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD12	7	0.61
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD13	7	0.61
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	13	0.61
(1,893)	1:40:C:VAL:HG21	1:42:C:LEU:H	12	0.61
(1,893)	1:40:C:VAL:HG22	1:42:C:LEU:H	12	0.61
(1,893)	1:40:C:VAL:HG23	1:42:C:LEU:H	12	0.61
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	2	0.61
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	5	0.61
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD21	17	0.61
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD22	17	0.61
(1,758)	1:127:B:ASN:H	1:128:B:LEU:HD23	17	0.61
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	3	0.61
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	15	0.61
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	15	0.61
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	15	0.61
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	15	0.61
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	15	0.61
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	15	0.61
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	15	0.61
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	15	0.61
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	15	0.61
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	15	0.61
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	15	0.61
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	15	0.61
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	15	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	15	0.61
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	15	0.61
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	1	0.61
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	8	0.61
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	8	0.61
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	8	0.61
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	15	0.6
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	4	0.6
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	18	0.6
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	18	0.6
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE1	7	0.6
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE2	7	0.6
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	16	0.6
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	11	0.6
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	16	0.6
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	13	0.6
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	19	0.6
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	11	0.6
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	11	0.6
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	12	0.6
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	12	0.6
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	2	0.6
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	4	0.6
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	3	0.6
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	3	0.6
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	3	0.6
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	3	0.6
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	3	0.6
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	3	0.6
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	3	0.6
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	3	0.6
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	3	0.6
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	16	0.6
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	3	0.6
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	15	0.6
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	7	0.6
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	2	0.6
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	12	0.6
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	6	0.6
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	17	0.6
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	17	0.6
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	13	0.59
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	13	0.59
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	14	0.59
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	14	0.59
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	14	0.59
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	15	0.59
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	15	0.59
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	15	0.59
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	7	0.59
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	19	0.59
(1,908)	1:43:C:ASP:H	1:63:C:THR:H	9	0.59
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	6	0.59
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	6	0.59
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	6	0.59
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	16	0.59
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	19	0.59
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	7	0.59
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	7	0.59
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	7	0.59
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD21	3	0.59
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD22	3	0.59
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD23	3	0.59
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD21	3	0.59
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD22	3	0.59
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD23	3	0.59
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	1	0.59
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	1	0.59
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	1	0.59
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	8	0.59
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	15	0.59
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	15	0.59
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	15	0.59
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	15	0.59
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	15	0.59
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	15	0.59
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	15	0.59
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	15	0.59
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	15	0.59
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	14	0.59
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	19	0.59
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	14	0.59
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	14	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	14	0.59
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	14	0.59
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	14	0.59
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	14	0.59
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	14	0.59
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	14	0.59
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	14	0.59
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	7	0.58
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	10	0.58
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	10	0.58
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	10	0.58
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	10	0.58
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	10	0.58
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	10	0.58
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	10	0.58
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	10	0.58
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	10	0.58
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	19	0.58
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	19	0.58
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	19	0.58
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	6	0.58
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE1	3	0.58
(1,1329)	1:50:D:GLN:H	1:56:D:TYR:HE2	3	0.58
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	19	0.58
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	20	0.58
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	10	0.58
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	6	0.58
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	20	0.58
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD11	3	0.58
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD12	3	0.58
(1,970)	1:56:C:TYR:HE1	1:98:C:LEU:HD13	3	0.58
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD11	3	0.58
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD12	3	0.58
(1,970)	1:56:C:TYR:HE2	1:98:C:LEU:HD13	3	0.58
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	14	0.58
(1,888)	1:39:C:GLU:H	1:67:C:SER:H	17	0.58
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	6	0.58
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	8	0.58
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	8	0.58
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	1	0.58
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	1	0.58
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	9	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	13	0.58
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	20	0.58
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	18	0.58
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	18	0.58
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	18	0.58
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	11	0.58
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	19	0.58
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	19	0.58
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	19	0.58
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD11	4	0.58
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD12	4	0.58
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD13	4	0.58
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD11	4	0.58
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD12	4	0.58
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD13	4	0.58
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD11	4	0.58
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD12	4	0.58
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD13	4	0.58
(1,348)	1:118:A:VAL:HG11	1:123:A:PHE:H	20	0.58
(1,348)	1:118:A:VAL:HG12	1:123:A:PHE:H	20	0.58
(1,348)	1:118:A:VAL:HG13	1:123:A:PHE:H	20	0.58
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	10	0.58
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	10	0.58
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	10	0.58
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	18	0.58
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	19	0.58
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	9	0.58
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG11	19	0.58
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG12	19	0.58
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG13	19	0.58
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	20	0.58
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	20	0.58
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	20	0.58
(1,5)	1:11:A:PHE:HD1	1:12:A:GLN:H	1	0.58
(1,5)	1:11:A:PHE:HD2	1:12:A:GLN:H	1	0.58
(1,1541)	1:126:D:LEU:HD11	1:127:D:ASN:H	13	0.57
(1,1541)	1:126:D:LEU:HD12	1:127:D:ASN:H	13	0.57
(1,1541)	1:126:D:LEU:HD13	1:127:D:ASN:H	13	0.57
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	12	0.57
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	12	0.57
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	12	0.57
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	18	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	18	0.57
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	18	0.57
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	18	0.57
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	18	0.57
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	18	0.57
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	18	0.57
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	18	0.57
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	18	0.57
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	16	0.57
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	16	0.57
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	16	0.57
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	16	0.57
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	16	0.57
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	16	0.57
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	16	0.57
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	16	0.57
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	16	0.57
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	12	0.57
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	13	0.57
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	13	0.57
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	3	0.57
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	10	0.57
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	6	0.57
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	3	0.57
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	8	0.57
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD11	20	0.57
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD12	20	0.57
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD13	20	0.57
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD11	20	0.57
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD12	20	0.57
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD13	20	0.57
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	14	0.57
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	8	0.57
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	8	0.57
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	8	0.57
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	10	0.57
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	10	0.57
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	10	0.57
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	10	0.57
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	10	0.57
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	10	0.57
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	10	0.57
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	10	0.57
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	17	0.57
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	5	0.57
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	5	0.57
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD21	20	0.57
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD22	20	0.57
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD23	20	0.57
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	14	0.57
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	14	0.57
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	12	0.56
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD21	9	0.56
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD22	9	0.56
(1,1354)	1:56:D:TYR:HD1	1:98:D:LEU:HD23	9	0.56
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD21	9	0.56
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD22	9	0.56
(1,1354)	1:56:D:TYR:HD2	1:98:D:LEU:HD23	9	0.56
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	5	0.56
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	5	0.56
(1,1107)	1:98:C:LEU:H	1:101:C:TYR:H	1	0.56
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	17	0.56
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	14	0.56
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	14	0.56
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	17	0.56
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	18	0.56
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	18	0.56
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	18	0.56
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	12	0.56
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	5	0.56
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	5	0.56
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	5	0.56
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	12	0.56
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	11	0.56
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	11	0.56
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	11	0.56
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	11	0.56
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	11	0.56
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	11	0.56
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	11	0.56
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	11	0.56
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	11	0.56
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	16	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	16	0.56
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	16	0.56
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	19	0.56
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	13	0.56
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	16	0.56
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	16	0.56
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	16	0.56
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	16	0.56
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	16	0.56
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	16	0.56
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	16	0.56
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	16	0.56
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	16	0.56
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG11	18	0.56
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG12	18	0.56
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG13	18	0.56
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD21	4	0.56
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD22	4	0.56
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD23	4	0.56
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	2	0.56
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	2	0.56
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	6	0.55
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	6	0.55
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	6	0.55
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	6	0.55
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	6	0.55
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	6	0.55
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	6	0.55
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	6	0.55
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	6	0.55
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	8	0.55
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	7	0.55
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	7	0.55
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	7	0.55
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	1	0.55
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	3	0.55
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	12	0.55
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	10	0.55
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	17	0.55
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	18	0.55
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	18	0.55
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	20	0.55
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	17	0.55
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	6	0.55
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	14	0.55
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	12	0.54
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	20	0.54
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	20	0.54
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	20	0.54
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	1	0.54
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	11	0.54
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	5	0.54
(1,1182)	1:135:C:ALA:H	1:138:C:MET:H	16	0.54
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	14	0.54
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	11	0.54
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	11	0.54
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	5	0.54
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	15	0.54
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	15	0.54
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	15	0.54
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	15	0.54
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	15	0.54
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	15	0.54
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	15	0.54
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	15	0.54
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	15	0.54
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	14	0.54
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	15	0.54
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	8	0.54
(1,686)	1:94:B:MET:HE1	1:95:B:ALA:H	17	0.54
(1,686)	1:94:B:MET:HE2	1:95:B:ALA:H	17	0.54
(1,686)	1:94:B:MET:HE3	1:95:B:ALA:H	17	0.54
(1,679)	1:92:B:THR:H	1:94:B:MET:H	17	0.54
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	13	0.54
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	13	0.54
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	6	0.54
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	6	0.54
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	6	0.54
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	6	0.54
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	6	0.54
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	6	0.54
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	6	0.54
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	6	0.54
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	3	0.54
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	16	0.54
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	16	0.54
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	16	0.54
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	7	0.54
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	19	0.54
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	11	0.54
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	11	0.54
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	11	0.54
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	11	0.54
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	11	0.54
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	11	0.54
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	11	0.54
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	11	0.54
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	11	0.54
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	15	0.54
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	13	0.54
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	13	0.54
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	13	0.54
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	11	0.54
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	17	0.53
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	17	0.53
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	7	0.53
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	7	0.53
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	7	0.53
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	7	0.53
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	7	0.53
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	7	0.53
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	7	0.53
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	7	0.53
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	7	0.53
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	10	0.53
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	10	0.53
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	10	0.53
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	10	0.53
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	20	0.53
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	20	0.53
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	20	0.53
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	20	0.53
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	11	0.53
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	20	0.53
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	5	0.53
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	10	0.53
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	12	0.53
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	17	0.53
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	16	0.53
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	16	0.53
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	16	0.53
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	16	0.53
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	16	0.53
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	16	0.53
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	16	0.53
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	16	0.53
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	16	0.53
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	11	0.53
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	11	0.53
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	11	0.53
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	2	0.53
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	2	0.53
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	11	0.53
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	5	0.53
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	17	0.53
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	10	0.53
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	20	0.53
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	12	0.53
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	17	0.53
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	16	0.53
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	9	0.53
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	9	0.53
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	9	0.53
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	3	0.52
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	3	0.52
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	13	0.52
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	12	0.52
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	12	0.52
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	5	0.52
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	14	0.52
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	9	0.52
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	13	0.52
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	2	0.52
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	17	0.52
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	15	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	15	0.52
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	15	0.52
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	15	0.52
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	15	0.52
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	15	0.52
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	15	0.52
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	15	0.52
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	15	0.52
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	9	0.52
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	1	0.52
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	16	0.52
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	10	0.52
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	10	0.52
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	10	0.52
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	9	0.51
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	9	0.51
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	9	0.51
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	9	0.51
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	9	0.51
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	9	0.51
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	13	0.51
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	2	0.51
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	2	0.51
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	2	0.51
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	2	0.51
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	2	0.51
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	2	0.51
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	2	0.51
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	2	0.51
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	2	0.51
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	12	0.51
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	2	0.51
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	15	0.51
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	1	0.51
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	4	0.51
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	8	0.51
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	12	0.51
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	16	0.51
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	1	0.51
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	16	0.51
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	16	0.51
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:92:B:THR:H	1:94:B:MET:H	7	0.51
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	9	0.51
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	9	0.51
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	9	0.51
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE1	19	0.51
(1,490)	1:40:B:VAL:HG21	1:74:B:PHE:HE2	19	0.51
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE1	19	0.51
(1,490)	1:40:B:VAL:HG22	1:74:B:PHE:HE2	19	0.51
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE1	19	0.51
(1,490)	1:40:B:VAL:HG23	1:74:B:PHE:HE2	19	0.51
(1,482)	1:40:B:VAL:HG11	1:42:B:LEU:H	11	0.51
(1,482)	1:40:B:VAL:HG12	1:42:B:LEU:H	11	0.51
(1,482)	1:40:B:VAL:HG13	1:42:B:LEU:H	11	0.51
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	6	0.51
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	6	0.51
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	6	0.51
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	5	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	14	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	14	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	14	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	14	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	14	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	14	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	14	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	14	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	14	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	20	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	20	0.51
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	20	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	20	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	20	0.51
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	20	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	20	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	20	0.51
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	20	0.51
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	8	0.51
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	15	0.51
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	20	0.5
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	20	0.5
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	20	0.5
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	20	0.5
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	20	0.5
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	16	0.5
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	4	0.5
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	4	0.5
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	4	0.5
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	13	0.5
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	20	0.5
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	20	0.5
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	18	0.5
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	12	0.5
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	17	0.5
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD11	3	0.5
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD12	3	0.5
(1,896)	1:41:C:LYS:H	1:42:C:LEU:HD13	3	0.5
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	3	0.5
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	11	0.5
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	3	0.5
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	3	0.5
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	7	0.5
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	7	0.5
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	5	0.5
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	11	0.5
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	20	0.5
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	20	0.5
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	20	0.5
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	20	0.5
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	20	0.5
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	20	0.5
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	20	0.5
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	20	0.5
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	20	0.5
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE1	20	0.5
(1,515)	1:44:B:LEU:HD21	1:133:B:PHE:HE2	20	0.5
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE1	20	0.5
(1,515)	1:44:B:LEU:HD22	1:133:B:PHE:HE2	20	0.5
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE1	20	0.5
(1,515)	1:44:B:LEU:HD23	1:133:B:PHE:HE2	20	0.5
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	11	0.5
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	11	0.5
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	11	0.5
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	11	0.5
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	11	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	11	0.5
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	11	0.5
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	11	0.5
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	11	0.5
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	17	0.5
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	17	0.5
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	10	0.5
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE1	19	0.5
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE2	19	0.5
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE3	19	0.5
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	20	0.5
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	9	0.5
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	1	0.5
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	10	0.49
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	10	0.49
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	10	0.49
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	10	0.49
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	10	0.49
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	10	0.49
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	10	0.49
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	10	0.49
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	10	0.49
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	2	0.49
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD11	7	0.49
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD12	7	0.49
(1,1286)	1:40:D:VAL:HG11	1:126:D:LEU:HD13	7	0.49
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD11	7	0.49
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD12	7	0.49
(1,1286)	1:40:D:VAL:HG12	1:126:D:LEU:HD13	7	0.49
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD11	7	0.49
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD12	7	0.49
(1,1286)	1:40:D:VAL:HG13	1:126:D:LEU:HD13	7	0.49
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	17	0.49
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	17	0.49
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	20	0.49
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	20	0.49
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	16	0.49
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	16	0.49
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	16	0.49
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	16	0.49
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	16	0.49
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	16	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	16	0.49
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	16	0.49
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	16	0.49
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	4	0.49
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	16	0.49
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	7	0.49
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	11	0.49
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	1	0.49
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	5	0.49
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	1	0.49
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	4	0.49
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	4	0.49
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	4	0.49
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	10	0.49
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	10	0.49
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	10	0.49
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	18	0.49
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	3	0.49
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE1	9	0.49
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE2	9	0.49
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE3	9	0.49
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	18	0.49
(1,532)	1:49:B:SER:H	1:59:B:VAL:H	19	0.49
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	15	0.49
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	15	0.49
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	15	0.49
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	15	0.49
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	15	0.49
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	15	0.49
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	15	0.49
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	15	0.49
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	15	0.49
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	8	0.49
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	8	0.49
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	8	0.49
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	4	0.49
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	4	0.49
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	4	0.49
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	4	0.49
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	4	0.49
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	4	0.49
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	4	0.49
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	4	0.49
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	20	0.49
(1,348)	1:118:A:VAL:HG11	1:123:A:PHE:H	4	0.49
(1,348)	1:118:A:VAL:HG12	1:123:A:PHE:H	4	0.49
(1,348)	1:118:A:VAL:HG13	1:123:A:PHE:H	4	0.49
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	17	0.49
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB1	8	0.49
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB2	8	0.49
(1,230)	1:68:A:LEU:HD21	1:73:A:ALA:HB3	8	0.49
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB1	8	0.49
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB2	8	0.49
(1,230)	1:68:A:LEU:HD22	1:73:A:ALA:HB3	8	0.49
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB1	8	0.49
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB2	8	0.49
(1,230)	1:68:A:LEU:HD23	1:73:A:ALA:HB3	8	0.49
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	3	0.49
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	18	0.49
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	18	0.49
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	18	0.49
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	18	0.49
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	18	0.49
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	18	0.49
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	18	0.49
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	18	0.49
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	18	0.49
(1,179)	1:59:A:VAL:HG21	1:81:A:GLY:H	8	0.49
(1,179)	1:59:A:VAL:HG22	1:81:A:GLY:H	8	0.49
(1,179)	1:59:A:VAL:HG23	1:81:A:GLY:H	8	0.49
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	13	0.49
(1,124)	1:44:A:LEU:HD21	1:133:A:PHE:HE1	19	0.49
(1,124)	1:44:A:LEU:HD21	1:133:A:PHE:HE2	19	0.49
(1,124)	1:44:A:LEU:HD22	1:133:A:PHE:HE1	19	0.49
(1,124)	1:44:A:LEU:HD22	1:133:A:PHE:HE2	19	0.49
(1,124)	1:44:A:LEU:HD23	1:133:A:PHE:HE1	19	0.49
(1,124)	1:44:A:LEU:HD23	1:133:A:PHE:HE2	19	0.49
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	16	0.49
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE1	5	0.48
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE2	5	0.48
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE1	5	0.48
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE2	5	0.48
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE1	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE2	5	0.48
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	20	0.48
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	8	0.48
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	8	0.48
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	13	0.48
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	13	0.48
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	13	0.48
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	17	0.48
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	17	0.48
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	17	0.48
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	18	0.48
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	11	0.48
(1,984)	1:60:C:LEU:H	1:80:C:GLN:H	14	0.48
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	3	0.48
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	6	0.48
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	10	0.48
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	5	0.48
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	5	0.48
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	5	0.48
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	5	0.48
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	5	0.48
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	5	0.48
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	5	0.48
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	5	0.48
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	5	0.48
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	5	0.48
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	5	0.48
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	5	0.48
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	18	0.48
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	18	0.48
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	18	0.48
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	1	0.48
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	15	0.48
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	18	0.48
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	19	0.48
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	17	0.48
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	15	0.48
(1,75)	1:31:A:VAL:HG11	1:32:A:PHE:H	8	0.48
(1,75)	1:31:A:VAL:HG12	1:32:A:PHE:H	8	0.48
(1,75)	1:31:A:VAL:HG13	1:32:A:PHE:H	8	0.48
(1,19)	1:14:A:GLN:H	1:84:A:PHE:H	7	0.48
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	10	0.47
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	10	0.47
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	10	0.47
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	10	0.47
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	10	0.47
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	4	0.47
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	2	0.47
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	2	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	3	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	3	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	3	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	8	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	8	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	8	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	17	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	17	0.47
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	17	0.47
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	18	0.47
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD11	2	0.47
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD12	2	0.47
(1,1302)	1:43:D:ASP:H	1:128:D:LEU:HD13	2	0.47
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	10	0.47
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	19	0.47
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	15	0.47
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	15	0.47
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	7	0.47
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	15	0.47
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	15	0.47
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	8	0.47
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	17	0.47
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	20	0.47
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	19	0.47
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	6	0.47
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	15	0.47
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	1	0.47
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	1	0.47
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	1	0.47
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	8	0.47
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	14	0.47
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	19	0.47
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	20	0.47
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	6	0.47
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	20	0.47
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	11	0.47
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	9	0.47
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	9	0.47
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	9	0.47
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	4	0.47
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	16	0.47
(1,229)	1:68:A:LEU:HD21	1:73:A:ALA:H	19	0.47
(1,229)	1:68:A:LEU:HD22	1:73:A:ALA:H	19	0.47
(1,229)	1:68:A:LEU:HD23	1:73:A:ALA:H	19	0.47
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	16	0.47
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	16	0.47
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	16	0.47
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	16	0.47
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	16	0.47
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	16	0.47
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	16	0.47
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	16	0.47
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	16	0.47
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	20	0.47
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	13	0.47
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	13	0.47
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	2	0.47
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	2	0.47
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	2	0.47
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	2	0.47
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	7	0.47
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	19	0.46
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	19	0.46
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	19	0.46
(1,1467)	1:92:D:THR:H	1:95:D:ALA:H	10	0.46
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	3	0.46
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE1	7	0.46
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE2	7	0.46
(1,1083)	1:91:C:GLY:H	1:94:C:MET:HE3	7	0.46
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	5	0.46
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	5	0.46
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	5	0.46
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	5	0.46
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	4	0.46
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	6	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	2	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	2	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	2	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	3	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	3	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	3	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	20	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	20	0.46
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	20	0.46
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	6	0.46
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	9	0.46
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	7	0.46
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	7	0.46
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	7	0.46
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	10	0.46
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	6	0.46
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	2	0.46
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE1	13	0.46
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE2	13	0.46
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE3	13	0.46
(1,131)	1:47:A:ALA:H	1:61:A:ARG:H	10	0.46
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	5	0.46
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	5	0.46
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	5	0.46
(1,8)	1:11:A:PHE:HE1	1:12:A:GLN:H	1	0.46
(1,8)	1:11:A:PHE:HE2	1:12:A:GLN:H	1	0.46
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	17	0.45
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	17	0.45
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	17	0.45
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	17	0.45
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	17	0.45
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	17	0.45
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	12	0.45
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	11	0.45
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	11	0.45
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	11	0.45
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	19	0.45
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	19	0.45
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	19	0.45
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	19	0.45
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	19	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	19	0.45
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	19	0.45
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	19	0.45
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	19	0.45
(1,1278)	1:36:D:TRP:HZ3	1:37:D:GLN:H	13	0.45
(1,1169)	1:131:C:VAL:HG11	1:133:C:PHE:H	18	0.45
(1,1169)	1:131:C:VAL:HG12	1:133:C:PHE:H	18	0.45
(1,1169)	1:131:C:VAL:HG13	1:133:C:PHE:H	18	0.45
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	6	0.45
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	9	0.45
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	19	0.45
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	18	0.45
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	7	0.45
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	4	0.45
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	4	0.45
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	4	0.45
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	4	0.45
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	4	0.45
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	4	0.45
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	4	0.45
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	4	0.45
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	4	0.45
(1,532)	1:49:B:SER:H	1:59:B:VAL:H	3	0.45
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	17	0.45
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD21	4	0.45
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD22	4	0.45
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD23	4	0.45
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD21	4	0.45
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD22	4	0.45
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD23	4	0.45
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD21	4	0.45
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD22	4	0.45
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD23	4	0.45
(1,348)	1:118:A:VAL:HG11	1:123:A:PHE:H	14	0.45
(1,348)	1:118:A:VAL:HG12	1:123:A:PHE:H	14	0.45
(1,348)	1:118:A:VAL:HG13	1:123:A:PHE:H	14	0.45
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	10	0.45
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	16	0.45
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	20	0.45
(1,177)	1:59:A:VAL:HG11	1:81:A:GLY:H	20	0.45
(1,177)	1:59:A:VAL:HG12	1:81:A:GLY:H	20	0.45
(1,177)	1:59:A:VAL:HG13	1:81:A:GLY:H	20	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	11	0.45
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	8	0.45
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	8	0.45
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	5	0.44
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	5	0.44
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	5	0.44
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	5	0.44
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	5	0.44
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	5	0.44
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	4	0.44
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	13	0.44
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	13	0.44
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	13	0.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD21	11	0.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD22	11	0.44
(1,1356)	1:56:D:TYR:HE1	1:98:D:LEU:HD23	11	0.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD21	11	0.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD22	11	0.44
(1,1356)	1:56:D:TYR:HE2	1:98:D:LEU:HD23	11	0.44
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	10	0.44
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	10	0.44
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	3	0.44
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	4	0.44
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	2	0.44
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	2	0.44
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	4	0.44
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	4	0.44
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	19	0.44
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	4	0.44
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	4	0.44
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	4	0.44
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	4	0.44
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	4	0.44
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	4	0.44
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	4	0.44
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	4	0.44
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	4	0.44
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	17	0.44
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	7	0.44
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	7	0.44
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	7	0.44
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	8	0.44
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	16	0.44
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	2	0.44
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	2	0.44
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	2	0.44
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	2	0.44
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	2	0.44
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	2	0.44
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	2	0.44
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	2	0.44
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	2	0.44
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	15	0.44
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	14	0.44
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	6	0.44
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	18	0.44
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	4	0.44
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	4	0.44
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	4	0.44
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	6	0.44
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	6	0.44
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	6	0.44
(1,532)	1:49:B:SER:H	1:59:B:VAL:H	7	0.44
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	16	0.44
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	16	0.44
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	16	0.44
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	16	0.44
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	16	0.44
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	16	0.44
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	16	0.44
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	16	0.44
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	16	0.44
(1,497)	1:42:B:LEU:HD11	1:43:B:ASP:H	4	0.44
(1,497)	1:42:B:LEU:HD12	1:43:B:ASP:H	4	0.44
(1,497)	1:42:B:LEU:HD13	1:43:B:ASP:H	4	0.44
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	5	0.44
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	12	0.44
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	4	0.44
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	9	0.44
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	14	0.44
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	5	0.44
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	4	0.44
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	4	0.44
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	4	0.44
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	4	0.44
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	4	0.44
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	4	0.44
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	4	0.44
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	4	0.44
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	17	0.44
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	8	0.44
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	9	0.44
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG11	6	0.44
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG12	6	0.44
(1,129)	1:47:A:ALA:H	1:58:A:VAL:HG13	6	0.44
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	18	0.44
(1,1569)	1:137:D:PHE:H	1:140:D:TYR:H	16	0.43
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	2	0.43
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	4	0.43
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	4	0.43
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	11	0.43
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	13	0.43
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	13	0.43
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	17	0.43
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	17	0.43
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	17	0.43
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	15	0.43
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	12	0.43
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	9	0.43
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	12	0.43
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	11	0.43
(1,888)	1:39:C:GLU:H	1:67:C:SER:H	8	0.43
(1,772)	1:135:B:ALA:HB1	1:136:B:LEU:HD21	17	0.43
(1,772)	1:135:B:ALA:HB1	1:136:B:LEU:HD22	17	0.43
(1,772)	1:135:B:ALA:HB1	1:136:B:LEU:HD23	17	0.43
(1,772)	1:135:B:ALA:HB2	1:136:B:LEU:HD21	17	0.43
(1,772)	1:135:B:ALA:HB2	1:136:B:LEU:HD22	17	0.43
(1,772)	1:135:B:ALA:HB2	1:136:B:LEU:HD23	17	0.43
(1,772)	1:135:B:ALA:HB3	1:136:B:LEU:HD21	17	0.43
(1,772)	1:135:B:ALA:HB3	1:136:B:LEU:HD22	17	0.43
(1,772)	1:135:B:ALA:HB3	1:136:B:LEU:HD23	17	0.43
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	11	0.43
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	9	0.43
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	13	0.43
(1,679)	1:92:B:THR:H	1:94:B:MET:H	19	0.43
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	13	0.43
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	13	0.43
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	13	0.43
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	15	0.43
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	15	0.43
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	15	0.43
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	11	0.43
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	5	0.43
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	3	0.43
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	9	0.43
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	11	0.43
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	2	0.43
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	11	0.43
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	11	0.43
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	11	0.43
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	15	0.43
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	19	0.43
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	20	0.42
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	6	0.42
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	9	0.42
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	9	0.42
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	18	0.42
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	18	0.42
(1,1282)	1:39:D:GLU:H	1:67:D:SER:H	10	0.42
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	13	0.42
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	13	0.42
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	14	0.42
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	16	0.42
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	16	0.42
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	1	0.42
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	1	0.42
(1,1094)	1:95:C:ALA:H	1:98:C:LEU:H	1	0.42
(1,1090)	1:94:C:MET:H	1:96:C:HIS:H	8	0.42
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	8	0.42
(1,899)	1:41:C:LYS:H	1:67:C:SER:H	13	0.42
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	15	0.42
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	16	0.42
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	8	0.42
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	4	0.42
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	17	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	1	0.42
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	4	0.42
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	3	0.42
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	4	0.42
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	4	0.42
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	2	0.42
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	5	0.42
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	9	0.42
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	9	0.42
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	9	0.42
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	9	0.42
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	9	0.42
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	9	0.42
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	9	0.42
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	9	0.42
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	9	0.42
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	7	0.42
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	12	0.42
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	18	0.42
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	5	0.42
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	18	0.42
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	12	0.42
(1,289)	1:95:A:ALA:H	1:98:A:LEU:H	8	0.42
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	4	0.42
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	4	0.42
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	4	0.42
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	18	0.42
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	18	0.42
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	18	0.42
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	18	0.42
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG11	1	0.41
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG12	1	0.41
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG13	1	0.41
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG11	1	0.41
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG12	1	0.41
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG13	1	0.41
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG11	1	0.41
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG12	1	0.41
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG13	1	0.41
(1,1566)	1:136:D:LEU:H	1:139:D:ASN:H	16	0.41
(1,1495)	1:100:D:ALA:H	1:102:D:CYS:H	10	0.41
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	8	0.41
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	15	0.41
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	1	0.41
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	1	0.41
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	10	0.41
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	3	0.41
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	20	0.41
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	10	0.41
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	11	0.41
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	11	0.41
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	11	0.41
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	11	0.41
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	11	0.41
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	11	0.41
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	11	0.41
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	11	0.41
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	11	0.41
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	13	0.41
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	1	0.41
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	1	0.41
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	20	0.41
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	17	0.41
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	19	0.41
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	1	0.41
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	2	0.41
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	20	0.41
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	8	0.41
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD1	2	0.41
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD2	2	0.41
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	8	0.41
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	20	0.41
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	16	0.41
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD11	13	0.41
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD12	13	0.41
(1,368)	1:131:A:VAL:HG11	1:136:A:LEU:HD13	13	0.41
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD11	13	0.41
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD12	13	0.41
(1,368)	1:131:A:VAL:HG12	1:136:A:LEU:HD13	13	0.41
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD11	13	0.41
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD12	13	0.41
(1,368)	1:131:A:VAL:HG13	1:136:A:LEU:HD13	13	0.41
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	16	0.41
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	16	0.41
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	16	0.41
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	7	0.41
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	3	0.41
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	19	0.41
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	19	0.41
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	19	0.41
(1,180)	1:59:A:VAL:HG21	1:82:A:GLY:H	8	0.41
(1,180)	1:59:A:VAL:HG22	1:82:A:GLY:H	8	0.41
(1,180)	1:59:A:VAL:HG23	1:82:A:GLY:H	8	0.41
(1,176)	1:59:A:VAL:HG11	1:80:A:GLN:H	20	0.41
(1,176)	1:59:A:VAL:HG12	1:80:A:GLN:H	20	0.41
(1,176)	1:59:A:VAL:HG13	1:80:A:GLN:H	20	0.41
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB1	17	0.41
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB2	17	0.41
(1,96)	1:39:A:GLU:H	1:66:A:ALA:HB3	17	0.41
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG11	13	0.4
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG12	13	0.4
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG13	13	0.4
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG21	13	0.4
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG22	13	0.4
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG23	13	0.4
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG11	13	0.4
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG12	13	0.4
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG13	13	0.4
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG21	13	0.4
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG22	13	0.4
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG23	13	0.4
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG11	13	0.4
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG12	13	0.4
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG13	13	0.4
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG21	13	0.4
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG22	13	0.4
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG23	13	0.4
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	13	0.4
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	2	0.4
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	16	0.4
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	9	0.4
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	6	0.4
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	7	0.4
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	2	0.4
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	2	0.4
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	2	0.4
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	9	0.4
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	9	0.4
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	16	0.4
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	1	0.4
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	3	0.4
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	5	0.4
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	1	0.4
(1,921)	1:45:C:ASP:H	1:63:C:THR:H	20	0.4
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	12	0.4
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	12	0.4
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	12	0.4
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	13	0.4
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	4	0.4
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	13	0.4
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	5	0.4
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	15	0.4
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	15	0.4
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	15	0.4
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	1	0.4
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD21	20	0.4
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD22	20	0.4
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD23	20	0.4
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD21	20	0.4
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD22	20	0.4
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD23	20	0.4
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD21	20	0.4
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD22	20	0.4
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD23	20	0.4
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	14	0.4
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	15	0.4
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	10	0.4
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	5	0.39
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	5	0.39
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	5	0.39
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	5	0.39
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	5	0.39
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	5	0.39
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	17	0.39
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	20	0.39
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	2	0.39
(1,1276)	1:36:D:TRP:HE1	1:39:D:GLU:H	10	0.39
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	3	0.39
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	12	0.39
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	9	0.39
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	9	0.39
(1,1201)	1:10:D:THR:H	1:87:D:ALA:H	15	0.39
(1,1178)	1:134:C:ASP:H	1:136:C:LEU:H	14	0.39
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	16	0.39
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	13	0.39
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	17	0.39
(1,1049)	1:74:C:PHE:HE1	1:126:C:LEU:HD11	9	0.39
(1,1049)	1:74:C:PHE:HE1	1:126:C:LEU:HD12	9	0.39
(1,1049)	1:74:C:PHE:HE1	1:126:C:LEU:HD13	9	0.39
(1,1049)	1:74:C:PHE:HE2	1:126:C:LEU:HD11	9	0.39
(1,1049)	1:74:C:PHE:HE2	1:126:C:LEU:HD12	9	0.39
(1,1049)	1:74:C:PHE:HE2	1:126:C:LEU:HD13	9	0.39
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	12	0.39
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	13	0.39
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	14	0.39
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	1	0.39
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	1	0.39
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	1	0.39
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	1	0.39
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	1	0.39
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	1	0.39
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	1	0.39
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	1	0.39
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	1	0.39
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	20	0.39
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	19	0.39
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	6	0.39
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	11	0.39
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	2	0.39
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	20	0.39
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	12	0.39
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	8	0.39
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	14	0.39
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	16	0.39
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	7	0.39
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	18	0.39
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	7	0.39
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	15	0.39
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	12	0.39
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	12	0.39
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG11	3	0.39
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG12	3	0.39
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG13	3	0.39
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	10	0.39
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	10	0.39
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	10	0.39
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	9	0.39
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	10	0.39
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	8	0.39
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	19	0.39
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	5	0.39
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	5	0.39
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	5	0.39
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	8	0.39
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	17	0.39
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	6	0.39
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	18	0.39
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	18	0.38
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD21	20	0.38
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD22	20	0.38
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD23	20	0.38
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD21	20	0.38
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD22	20	0.38
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD23	20	0.38
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD21	20	0.38
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD22	20	0.38
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD23	20	0.38
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	12	0.38
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	12	0.38
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	12	0.38
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	12	0.38
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	12	0.38
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	12	0.38
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	12	0.38
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	12	0.38
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	12	0.38
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	16	0.38
(1,1282)	1:39:D:GLU:H	1:67:D:SER:H	3	0.38
(1,1247)	1:28:D:ALA:H	1:30:D:HIS:H	18	0.38
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	20	0.38
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	20	0.38
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	8	0.38
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	14	0.38
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	6	0.38
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	6	0.38
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	16	0.38
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	16	0.38
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	17	0.38
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	17	0.38
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	4	0.38
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	12	0.38
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	3	0.38
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	8	0.38
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	1	0.38
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD11	17	0.38
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD12	17	0.38
(1,1023)	1:66:C:ALA:HB1	1:126:C:LEU:HD13	17	0.38
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD11	17	0.38
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD12	17	0.38
(1,1023)	1:66:C:ALA:HB2	1:126:C:LEU:HD13	17	0.38
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD11	17	0.38
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD12	17	0.38
(1,1023)	1:66:C:ALA:HB3	1:126:C:LEU:HD13	17	0.38
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	17	0.38
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	18	0.38
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	3	0.38
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	4	0.38
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	10	0.38
(1,899)	1:41:C:LYS:H	1:67:C:SER:H	10	0.38
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	8	0.38
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	2	0.38
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	7	0.38
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	20	0.38
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	8	0.38
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	4	0.38
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	16	0.38
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	20	0.38
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	16	0.38
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	14	0.38
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	7	0.38
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	15	0.38
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	17	0.38
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD21	1	0.38
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD22	1	0.38
(1,352)	1:118:A:VAL:HG21	1:126:A:LEU:HD23	1	0.38
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD21	1	0.38
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD22	1	0.38
(1,352)	1:118:A:VAL:HG22	1:126:A:LEU:HD23	1	0.38
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD21	1	0.38
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD22	1	0.38
(1,352)	1:118:A:VAL:HG23	1:126:A:LEU:HD23	1	0.38
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	13	0.38
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	9	0.38
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	8	0.38
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	20	0.38
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	20	0.38
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	20	0.38
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	20	0.38
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	20	0.38
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	20	0.38
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	20	0.38
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	20	0.38
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	20	0.38
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	17	0.38
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	17	0.38
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	17	0.38
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	17	0.38
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	17	0.38
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	17	0.38
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	17	0.38
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	17	0.38
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	17	0.38
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	18	0.38
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	20	0.38
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	20	0.38
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	20	0.38
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	20	0.38
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	15	0.37
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	15	0.37
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD21	17	0.37
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD22	17	0.37
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD23	17	0.37
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD21	17	0.37
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD22	17	0.37
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD23	17	0.37
(1,1414)	1:68:D:LEU:H	1:71:D:GLU:H	7	0.37
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	10	0.37
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	17	0.37
(1,1277)	1:36:D:TRP:HE1	1:69:D:GLY:H	7	0.37
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	1	0.37
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	1	0.37
(1,1201)	1:10:D:THR:H	1:87:D:ALA:H	11	0.37
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	11	0.37
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	11	0.37
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	11	0.37
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	3	0.37
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	5	0.37
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	18	0.37
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	13	0.37
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	13	0.37
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	3	0.37
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	8	0.37
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	2	0.37
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	2	0.37
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	4	0.37
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	14	0.37
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	15	0.37
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	12	0.37
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	13	0.37
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	11	0.37
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	18	0.37
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	12	0.37
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	1	0.37
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	14	0.37
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	18	0.37
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	18	0.37
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	18	0.37
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	18	0.37
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	18	0.37
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	18	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	18	0.37
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	18	0.37
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	18	0.37
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	18	0.37
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	16	0.37
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	2	0.37
(1,305)	1:98:A:LEU:HD11	1:99:A:GLY:H	13	0.37
(1,305)	1:98:A:LEU:HD12	1:99:A:GLY:H	13	0.37
(1,305)	1:98:A:LEU:HD13	1:99:A:GLY:H	13	0.37
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	1	0.37
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	11	0.37
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	14	0.37
(1,225)	1:68:A:LEU:H	1:72:A:THR:H	7	0.37
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	8	0.37
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	19	0.37
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	15	0.37
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD11	16	0.37
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD12	16	0.37
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD13	16	0.37
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD11	16	0.37
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD12	16	0.37
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD13	16	0.37
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD11	16	0.37
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD12	16	0.37
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD13	16	0.37
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	5	0.37
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	5	0.37
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	5	0.37
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	5	0.37
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	5	0.37
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	5	0.37
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	5	0.37
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	5	0.37
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	5	0.37
(1,176)	1:59:A:VAL:HG11	1:80:A:GLN:H	9	0.37
(1,176)	1:59:A:VAL:HG12	1:80:A:GLN:H	9	0.37
(1,176)	1:59:A:VAL:HG13	1:80:A:GLN:H	9	0.37
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	13	0.37
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	10	0.37
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	17	0.37
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	7	0.37
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	15	0.36
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	15	0.36
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	15	0.36
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	15	0.36
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	15	0.36
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	8	0.36
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD11	17	0.36
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD12	17	0.36
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD13	17	0.36
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD11	17	0.36
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD12	17	0.36
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD13	17	0.36
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	9	0.36
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	9	0.36
(1,1308)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	12	0.36
(1,1308)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	12	0.36
(1,1308)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	12	0.36
(1,1308)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	12	0.36
(1,1308)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	12	0.36
(1,1308)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	12	0.36
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	8	0.36
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	5	0.36
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	20	0.36
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	13	0.36
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	1	0.36
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	1	0.36
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	5	0.36
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	5	0.36
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	13	0.36
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	12	0.36
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	8	0.36
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	13	0.36
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	6	0.36
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	17	0.36
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	2	0.36
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	2	0.36
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	2	0.36
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	9	0.36
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	14	0.36
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	5	0.36
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	18	0.36
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	19	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	6	0.36
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	6	0.36
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	8	0.36
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD21	4	0.36
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD22	4	0.36
(1,600)	1:64:B:VAL:HG11	1:126:B:LEU:HD23	4	0.36
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD21	4	0.36
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD22	4	0.36
(1,600)	1:64:B:VAL:HG12	1:126:B:LEU:HD23	4	0.36
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD21	4	0.36
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD22	4	0.36
(1,600)	1:64:B:VAL:HG13	1:126:B:LEU:HD23	4	0.36
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	3	0.36
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	11	0.36
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	11	0.36
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	11	0.36
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	8	0.36
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	17	0.36
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	17	0.36
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	17	0.36
(1,475)	1:36:B:TRP:HE1	1:39:B:GLU:H	17	0.36
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	14	0.36
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	9	0.36
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	5	0.36
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	5	0.36
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	4	0.36
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	4	0.36
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	6	0.36
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	19	0.36
(1,184)	1:60:A:LEU:HD11	1:61:A:ARG:H	17	0.36
(1,184)	1:60:A:LEU:HD12	1:61:A:ARG:H	17	0.36
(1,184)	1:60:A:LEU:HD13	1:61:A:ARG:H	17	0.36
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	20	0.36
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	12	0.36
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	18	0.36
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	15	0.36
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	16	0.35
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	16	0.35
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	16	0.35
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	16	0.35
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	16	0.35
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG11	11	0.35
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG12	11	0.35
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG13	11	0.35
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG11	11	0.35
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG12	11	0.35
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG13	11	0.35
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG11	11	0.35
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG12	11	0.35
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG13	11	0.35
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	3	0.35
(1,1495)	1:100:D:ALA:H	1:102:D:CYS:H	19	0.35
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	20	0.35
(1,1334)	1:51:D:LEU:H	1:57:D:GLU:H	16	0.35
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	16	0.35
(1,1323)	1:49:D:SER:H	1:56:D:TYR:HD1	17	0.35
(1,1323)	1:49:D:SER:H	1:56:D:TYR:HD2	17	0.35
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	4	0.35
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	8	0.35
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	20	0.35
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE1	10	0.35
(1,1285)	1:40:D:VAL:HG11	1:74:D:PHE:HE2	10	0.35
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE1	10	0.35
(1,1285)	1:40:D:VAL:HG12	1:74:D:PHE:HE2	10	0.35
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE1	10	0.35
(1,1285)	1:40:D:VAL:HG13	1:74:D:PHE:HE2	10	0.35
(1,1164)	1:126:C:LEU:HD21	1:128:C:LEU:H	10	0.35
(1,1164)	1:126:C:LEU:HD22	1:128:C:LEU:H	10	0.35
(1,1164)	1:126:C:LEU:HD23	1:128:C:LEU:H	10	0.35
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	5	0.35
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	6	0.35
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	18	0.35
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	19	0.35
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	18	0.35
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	9	0.35
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	9	0.35
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	9	0.35
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	9	0.35
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	9	0.35
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	9	0.35
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	9	0.35
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	9	0.35
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	13	0.35
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	6	0.35
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	14	0.35
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	19	0.35
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	3	0.35
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	9	0.35
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	14	0.35
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	3	0.35
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	1	0.35
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	7	0.35
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	16	0.35
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	16	0.35
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	16	0.35
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	16	0.35
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	16	0.35
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	16	0.35
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	16	0.35
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	16	0.35
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	16	0.35
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	16	0.35
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	16	0.35
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	16	0.35
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	17	0.35
(1,479)	1:39:B:GLU:H	1:67:B:SER:H	19	0.35
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	13	0.35
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	13	0.35
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	13	0.35
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	2	0.35
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	14	0.35
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	17	0.35
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	6	0.35
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	2	0.35
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB1	14	0.35
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB2	14	0.35
(1,187)	1:60:A:LEU:HD21	1:110:A:ALA:HB3	14	0.35
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB1	14	0.35
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB2	14	0.35
(1,187)	1:60:A:LEU:HD22	1:110:A:ALA:HB3	14	0.35
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB1	14	0.35
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB2	14	0.35
(1,187)	1:60:A:LEU:HD23	1:110:A:ALA:HB3	14	0.35
(1,164)	1:56:A:TYR:H	1:86:A:ILE:H	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	2	0.35
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	14	0.35
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	13	0.35
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	11	0.35
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	11	0.35
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	11	0.35
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	1	0.34
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	1	0.34
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	1	0.34
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	1	0.34
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	1	0.34
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	1	0.34
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	18	0.34
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	18	0.34
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	18	0.34
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	18	0.34
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	18	0.34
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	18	0.34
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	12	0.34
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	14	0.34
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	5	0.34
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	5	0.34
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	5	0.34
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	3	0.34
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	5	0.34
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	10	0.34
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	18	0.34
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	19	0.34
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	16	0.34
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	4	0.34
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	7	0.34
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	10	0.34
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	3	0.34
(1,908)	1:43:C:ASP:H	1:63:C:THR:H	4	0.34
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	5	0.34
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	7	0.34
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	7	0.34
(1,797)	1:11:C:PHE:HD1	1:12:C:GLN:H	17	0.34
(1,797)	1:11:C:PHE:HD2	1:12:C:GLN:H	17	0.34
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	5	0.34
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	2	0.34
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	8	0.34
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	8	0.34
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	10	0.34
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	11	0.34
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	14	0.34
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	10	0.34
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	1	0.34
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	16	0.34
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	1	0.34
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	1	0.34
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	1	0.34
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	15	0.34
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	19	0.34
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	19	0.34
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	19	0.34
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	19	0.34
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	19	0.34
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	19	0.34
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	19	0.34
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	19	0.34
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	19	0.34
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD21	2	0.34
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD22	2	0.34
(1,487)	1:40:B:VAL:HG11	1:128:B:LEU:HD23	2	0.34
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD21	2	0.34
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD22	2	0.34
(1,487)	1:40:B:VAL:HG12	1:128:B:LEU:HD23	2	0.34
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD21	2	0.34
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD22	2	0.34
(1,487)	1:40:B:VAL:HG13	1:128:B:LEU:HD23	2	0.34
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	9	0.34
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	9	0.34
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	9	0.34
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	6	0.34
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	13	0.34
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	2	0.34
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	20	0.34
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	14	0.34
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	5	0.34
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	7	0.34
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	4	0.34
(1,177)	1:59:A:VAL:HG11	1:81:A:GLY:H	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:59:A:VAL:HG12	1:81:A:GLY:H	9	0.34
(1,177)	1:59:A:VAL:HG13	1:81:A:GLY:H	9	0.34
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	3	0.34
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	6	0.34
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	20	0.34
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	20	0.34
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	5	0.34
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	7	0.33
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	7	0.33
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	7	0.33
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	7	0.33
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	7	0.33
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	7	0.33
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG11	4	0.33
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG12	4	0.33
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG13	4	0.33
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG11	4	0.33
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG12	4	0.33
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG13	4	0.33
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG11	4	0.33
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG12	4	0.33
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG13	4	0.33
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	19	0.33
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	9	0.33
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	2	0.33
(1,1472)	1:94:D:MET:H	1:96:D:HIS:H	15	0.33
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	6	0.33
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	6	0.33
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD11	17	0.33
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD12	17	0.33
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD13	17	0.33
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD11	17	0.33
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD12	17	0.33
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD13	17	0.33
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	11	0.33
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	11	0.33
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	11	0.33
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	11	0.33
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	11	0.33
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	11	0.33
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	7	0.33
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	17	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	5	0.33
(1,1307)	1:44:D:LEU:HD21	1:45:D:ASP:H	13	0.33
(1,1307)	1:44:D:LEU:HD22	1:45:D:ASP:H	13	0.33
(1,1307)	1:44:D:LEU:HD23	1:45:D:ASP:H	13	0.33
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	4	0.33
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD11	2	0.33
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD12	2	0.33
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD13	2	0.33
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD11	2	0.33
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD12	2	0.33
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD13	2	0.33
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD11	2	0.33
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD12	2	0.33
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD13	2	0.33
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	2	0.33
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	2	0.33
(1,1090)	1:94:C:MET:H	1:96:C:HIS:H	4	0.33
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	2	0.33
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	4	0.33
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	13	0.33
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	18	0.33
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	1	0.33
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	1	0.33
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	1	0.33
(1,791)	1:9:C:MET:H	1:89:C:ILE:H	2	0.33
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	13	0.33
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	7	0.33
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	3	0.33
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	7	0.33
(1,686)	1:94:B:MET:HE1	1:95:B:ALA:H	14	0.33
(1,686)	1:94:B:MET:HE2	1:95:B:ALA:H	14	0.33
(1,686)	1:94:B:MET:HE3	1:95:B:ALA:H	14	0.33
(1,679)	1:92:B:THR:H	1:94:B:MET:H	10	0.33
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	19	0.33
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	3	0.33
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	3	0.33
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	3	0.33
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	3	0.33
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	3	0.33
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	3	0.33
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	3	0.33
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	3	0.33
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	16	0.33
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	4	0.33
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	13	0.33
(1,448)	1:28:B:ALA:H	1:30:B:HIS:H	19	0.33
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	13	0.33
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	17	0.33
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	14	0.33
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	16	0.33
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	13	0.33
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	14	0.33
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	15	0.33
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	1	0.33
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	3	0.33
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	1	0.33
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	7	0.33
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	8	0.33
(1,119)	1:44:A:LEU:HD11	1:46:A:THR:H	3	0.33
(1,119)	1:44:A:LEU:HD12	1:46:A:THR:H	3	0.33
(1,119)	1:44:A:LEU:HD13	1:46:A:THR:H	3	0.33
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	6	0.33
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	6	0.33
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	6	0.33
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG11	6	0.32
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG12	6	0.32
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG13	6	0.32
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG11	6	0.32
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG12	6	0.32
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG13	6	0.32
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG11	6	0.32
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG12	6	0.32
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG13	6	0.32
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG11	14	0.32
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG12	14	0.32
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG13	14	0.32
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG11	14	0.32
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG12	14	0.32
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG13	14	0.32
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG11	14	0.32
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG12	14	0.32
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG13	14	0.32
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE1	17	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE2	17	0.32
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE3	17	0.32
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE1	17	0.32
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE2	17	0.32
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE3	17	0.32
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE1	17	0.32
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE2	17	0.32
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE3	17	0.32
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	16	0.32
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	20	0.32
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	20	0.32
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	20	0.32
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	20	0.32
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	20	0.32
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	20	0.32
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	20	0.32
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	20	0.32
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	20	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	2	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	2	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	2	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	6	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	6	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	6	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	18	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	18	0.32
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	18	0.32
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	15	0.32
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	18	0.32
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	8	0.32
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	3	0.32
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	3	0.32
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	9	0.32
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	1	0.32
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	14	0.32
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	5	0.32
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	11	0.32
(1,961)	1:55:C:VAL:H	1:86:C:ILE:H	12	0.32
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	10	0.32
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	15	0.32
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	11	0.32
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:41:C:LYS:H	1:67:C:SER:H	7	0.32
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	7	0.32
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	17	0.32
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	5	0.32
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	12	0.32
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	1	0.32
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	14	0.32
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	17	0.32
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	9	0.32
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	17	0.32
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	14	0.32
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	15	0.32
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	10	0.32
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	6	0.32
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	9	0.32
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	12	0.32
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	14	0.32
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	19	0.32
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	14	0.32
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	14	0.32
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	14	0.32
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	12	0.32
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	20	0.32
(1,289)	1:95:A:ALA:H	1:98:A:LEU:H	17	0.32
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	9	0.32
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	9	0.32
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	15	0.32
(1,221)	1:67:A:SER:H	1:73:A:ALA:H	2	0.32
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	1	0.32
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	13	0.32
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	17	0.32
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	12	0.32
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG11	8	0.31
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG12	8	0.31
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG13	8	0.31
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG11	8	0.31
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG12	8	0.31
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG13	8	0.31
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG11	8	0.31
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG12	8	0.31
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG13	8	0.31
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	14	0.31
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	14	0.31
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	14	0.31
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	14	0.31
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	14	0.31
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	11	0.31
(1,1490)	1:99:D:GLY:H	1:100:D:ALA:H	11	0.31
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	5	0.31
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB1	10	0.31
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB2	10	0.31
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB3	10	0.31
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	1	0.31
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	1	0.31
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	1	0.31
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	15	0.31
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	4	0.31
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	3	0.31
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD11	18	0.31
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD12	18	0.31
(1,1295)	1:42:D:LEU:HD21	1:128:D:LEU:HD13	18	0.31
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD11	18	0.31
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD12	18	0.31
(1,1295)	1:42:D:LEU:HD22	1:128:D:LEU:HD13	18	0.31
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD11	18	0.31
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD12	18	0.31
(1,1295)	1:42:D:LEU:HD23	1:128:D:LEU:HD13	18	0.31
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	3	0.31
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	3	0.31
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	3	0.31
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	3	0.31
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	3	0.31
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	3	0.31
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	3	0.31
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	3	0.31
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	3	0.31
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	6	0.31
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	19	0.31
(1,1185)	1:136:C:LEU:H	1:138:C:MET:H	6	0.31
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	14	0.31
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	14	0.31
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	14	0.31
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	1	0.31
(1,1088)	1:93:C:GLN:H	1:96:C:HIS:H	8	0.31
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	10	0.31
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	14	0.31
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	3	0.31
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	8	0.31
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	20	0.31
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	14	0.31
(1,763)	1:133:B:PHE:H	1:135:B:ALA:H	6	0.31
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	16	0.31
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	8	0.31
(1,679)	1:92:B:THR:H	1:94:B:MET:H	1	0.31
(1,679)	1:92:B:THR:H	1:94:B:MET:H	11	0.31
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	6	0.31
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	3	0.31
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	13	0.31
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	6	0.31
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	6	0.31
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	6	0.31
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	12	0.31
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	18	0.31
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	12	0.31
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	12	0.31
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	12	0.31
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	12	0.31
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	12	0.31
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	12	0.31
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	12	0.31
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	12	0.31
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	12	0.31
(1,595)	1:64:B:VAL:H	1:76:B:CYS:H	5	0.31
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	15	0.31
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	14	0.31
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG21	5	0.31
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG22	5	0.31
(1,505)	1:42:B:LEU:HD21	1:131:B:VAL:HG23	5	0.31
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG21	5	0.31
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG22	5	0.31
(1,505)	1:42:B:LEU:HD22	1:131:B:VAL:HG23	5	0.31
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG21	5	0.31
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG22	5	0.31
(1,505)	1:42:B:LEU:HD23	1:131:B:VAL:HG23	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD21	18	0.31
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD22	18	0.31
(1,501)	1:42:B:LEU:HD11	1:128:B:LEU:HD23	18	0.31
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD21	18	0.31
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD22	18	0.31
(1,501)	1:42:B:LEU:HD12	1:128:B:LEU:HD23	18	0.31
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD21	18	0.31
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD22	18	0.31
(1,501)	1:42:B:LEU:HD13	1:128:B:LEU:HD23	18	0.31
(1,481)	1:40:B:VAL:HG11	1:41:B:LYS:H	20	0.31
(1,481)	1:40:B:VAL:HG12	1:41:B:LYS:H	20	0.31
(1,481)	1:40:B:VAL:HG13	1:41:B:LYS:H	20	0.31
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	4	0.31
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD21	5	0.31
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD22	5	0.31
(1,286)	1:94:A:MET:HE1	1:98:A:LEU:HD23	5	0.31
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD21	5	0.31
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD22	5	0.31
(1,286)	1:94:A:MET:HE2	1:98:A:LEU:HD23	5	0.31
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD21	5	0.31
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD22	5	0.31
(1,286)	1:94:A:MET:HE3	1:98:A:LEU:HD23	5	0.31
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	7	0.31
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	7	0.31
(1,103)	1:41:A:LYS:H	1:65:A:THR:H	18	0.31
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	10	0.31
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	10	0.31
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	10	0.31
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	10	0.31
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG21	7	0.3
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG22	7	0.3
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG23	7	0.3
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG21	7	0.3
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG22	7	0.3
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG23	7	0.3
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	18	0.3
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	18	0.3
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	18	0.3
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	18	0.3
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	18	0.3
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	18	0.3
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	3	0.3
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	3	0.3
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	3	0.3
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	3	0.3
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	3	0.3
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	16	0.3
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	16	0.3
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	16	0.3
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	16	0.3
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	16	0.3
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	16	0.3
(1,1569)	1:137:D:PHE:H	1:140:D:TYR:H	18	0.3
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	14	0.3
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	15	0.3
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	16	0.3
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	17	0.3
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	7	0.3
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	16	0.3
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	3	0.3
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	3	0.3
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	12	0.3
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	12	0.3
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	16	0.3
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	8	0.3
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	1	0.3
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	7	0.3
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	10	0.3
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	9	0.3
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	12	0.3
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	12	0.3
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	6	0.3
(1,908)	1:43:C:ASP:H	1:63:C:THR:H	6	0.3
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	2	0.3
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	4	0.3
(1,790)	1:9:C:MET:H	1:10:C:THR:H	13	0.3
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	8	0.3
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	9	0.3
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	12	0.3
(1,697)	1:97:B:CYS:H	1:99:B:GLY:H	12	0.3
(1,686)	1:94:B:MET:HE1	1:95:B:ALA:H	3	0.3
(1,686)	1:94:B:MET:HE2	1:95:B:ALA:H	3	0.3
(1,686)	1:94:B:MET:HE3	1:95:B:ALA:H	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:94:B:MET:H	1:97:B:CYS:H	10	0.3
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	1	0.3
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	15	0.3
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	2	0.3
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	10	0.3
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	10	0.3
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	10	0.3
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	3	0.3
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	19	0.3
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	13	0.3
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	10	0.3
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	12	0.3
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	12	0.3
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	12	0.3
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	12	0.3
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	12	0.3
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	12	0.3
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	12	0.3
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	12	0.3
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	12	0.3
(1,479)	1:39:B:GLU:H	1:67:B:SER:H	7	0.3
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	9	0.3
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	20	0.3
(1,329)	1:112:A:GLU:H	1:109:C:TYR:HE1	19	0.3
(1,329)	1:112:A:GLU:H	1:109:C:TYR:HE2	19	0.3
(1,305)	1:98:A:LEU:HD11	1:99:A:GLY:H	18	0.3
(1,305)	1:98:A:LEU:HD12	1:99:A:GLY:H	18	0.3
(1,305)	1:98:A:LEU:HD13	1:99:A:GLY:H	18	0.3
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	8	0.3
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	3	0.3
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	8	0.3
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	8	0.3
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	8	0.3
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	13	0.3
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	1	0.3
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	10	0.3
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD11	17	0.3
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD12	17	0.3
(1,194)	1:62:A:VAL:HG11	1:128:A:LEU:HD13	17	0.3
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD11	17	0.3
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD12	17	0.3
(1,194)	1:62:A:VAL:HG12	1:128:A:LEU:HD13	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD11	17	0.3
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD12	17	0.3
(1,194)	1:62:A:VAL:HG13	1:128:A:LEU:HD13	17	0.3
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	3	0.3
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	19	0.3
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	2	0.29
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	2	0.29
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	2	0.29
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	2	0.29
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	2	0.29
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	2	0.29
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD11	11	0.29
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD12	11	0.29
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD13	11	0.29
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD11	11	0.29
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD12	11	0.29
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD13	11	0.29
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD11	11	0.29
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD12	11	0.29
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD13	11	0.29
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG11	7	0.29
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG12	7	0.29
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG13	7	0.29
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG11	7	0.29
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG12	7	0.29
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG13	7	0.29
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG11	7	0.29
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG12	7	0.29
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG13	7	0.29
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	12	0.29
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	12	0.29
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	12	0.29
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	20	0.29
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD11	8	0.29
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD12	8	0.29
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD13	8	0.29
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD11	8	0.29
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD12	8	0.29
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD13	8	0.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	19	0.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	19	0.29
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	12	0.29
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	11	0.29
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	11	0.29
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	14	0.29
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	14	0.29
(1,1189)	1:137:C:PHE:H	1:140:C:TYR:H	16	0.29
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	8	0.29
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	20	0.29
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	2	0.29
(1,1107)	1:98:C:LEU:H	1:101:C:TYR:H	3	0.29
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	6	0.29
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	8	0.29
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	18	0.29
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	16	0.29
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	3	0.29
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD21	15	0.29
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD22	15	0.29
(1,1010)	1:64:C:VAL:HG21	1:126:C:LEU:HD23	15	0.29
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD21	15	0.29
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD22	15	0.29
(1,1010)	1:64:C:VAL:HG22	1:126:C:LEU:HD23	15	0.29
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD21	15	0.29
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD22	15	0.29
(1,1010)	1:64:C:VAL:HG23	1:126:C:LEU:HD23	15	0.29
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	2	0.29
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	2	0.29
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	7	0.29
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	1	0.29
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	15	0.29
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	18	0.29
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	11	0.29
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	12	0.29
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	17	0.29
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	17	0.29
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	11	0.29
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	11	0.29
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	3	0.29
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	4	0.29
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	5	0.29
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	17	0.29
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	11	0.29
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	13	0.29
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	13	0.29
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	13	0.29
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	1	0.29
(1,536)	1:51:B:LEU:H	1:55:B:VAL:H	11	0.29
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	11	0.29
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	17	0.29
(1,382)	1:136:A:LEU:H	1:138:A:MET:H	12	0.29
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	7	0.29
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	7	0.29
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	7	0.29
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	8	0.29
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	9	0.29
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	10	0.29
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	10	0.29
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	10	0.29
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	18	0.29
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	8	0.29
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	6	0.29
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	12	0.29
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	12	0.29
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG21	13	0.29
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG22	13	0.29
(1,186)	1:60:A:LEU:HD21	1:62:A:VAL:HG23	13	0.29
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG21	13	0.29
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG22	13	0.29
(1,186)	1:60:A:LEU:HD22	1:62:A:VAL:HG23	13	0.29
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG21	13	0.29
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG22	13	0.29
(1,186)	1:60:A:LEU:HD23	1:62:A:VAL:HG23	13	0.29
(1,183)	1:60:A:LEU:H	1:82:A:GLY:H	5	0.29
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	3	0.29
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	3	0.29
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	11	0.29
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	12	0.29
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	10	0.29
(1,131)	1:47:A:ALA:H	1:61:A:ARG:H	16	0.29
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	14	0.29
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	18	0.29
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	4	0.28
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	4	0.28
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	4	0.28
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	4	0.28
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	4	0.28
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	5	0.28
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	5	0.28
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	5	0.28
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	5	0.28
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	5	0.28
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	5	0.28
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	6	0.28
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	6	0.28
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	6	0.28
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	6	0.28
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	6	0.28
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	6	0.28
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD11	19	0.28
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD12	19	0.28
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD13	19	0.28
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD11	19	0.28
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD12	19	0.28
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD13	19	0.28
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD11	19	0.28
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD12	19	0.28
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD13	19	0.28
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	1	0.28
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	1	0.28
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	1	0.28
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	1	0.28
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	1	0.28
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	1	0.28
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD11	15	0.28
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD12	15	0.28
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD13	15	0.28
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD11	15	0.28
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD12	15	0.28
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD13	15	0.28
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD11	15	0.28
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD12	15	0.28
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD13	15	0.28
(1,1542)	1:126:D:LEU:HD11	1:128:D:LEU:H	6	0.28
(1,1542)	1:126:D:LEU:HD12	1:128:D:LEU:H	6	0.28
(1,1542)	1:126:D:LEU:HD13	1:128:D:LEU:H	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	1	0.28
(1,1471)	1:94:D:MET:H	1:95:D:ALA:H	10	0.28
(1,1467)	1:92:D:THR:H	1:95:D:ALA:H	7	0.28
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	1	0.28
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	11	0.28
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	14	0.28
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	18	0.28
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	18	0.28
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	18	0.28
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	18	0.28
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	18	0.28
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	18	0.28
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	18	0.28
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	18	0.28
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	18	0.28
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	6	0.28
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	16	0.28
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	16	0.28
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	16	0.28
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	16	0.28
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	16	0.28
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	16	0.28
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	16	0.28
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	16	0.28
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	16	0.28
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	14	0.28
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	15	0.28
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	15	0.28
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	17	0.28
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	17	0.28
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	13	0.28
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	15	0.28
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	5	0.28
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	14	0.28
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	14	0.28
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	13	0.28
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	13	0.28
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	17	0.28
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	10	0.28
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	8	0.28
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	14	0.28
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	2	0.28
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	5	0.28
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	8	0.28
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	8	0.28
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	8	0.28
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	8	0.28
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	20	0.28
(1,1030)	1:68:C:LEU:H	1:73:C:ALA:H	8	0.28
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	4	0.28
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	12	0.28
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	4	0.28
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	10	0.28
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	10	0.28
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	10	0.28
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	10	0.28
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	10	0.28
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	10	0.28
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	10	0.28
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	10	0.28
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	10	0.28
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	3	0.28
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	3	0.28
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	3	0.28
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	4	0.28
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	4	0.28
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	4	0.28
(1,888)	1:39:C:GLU:H	1:67:C:SER:H	6	0.28
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	9	0.28
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	20	0.28
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	17	0.28
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	12	0.28
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	16	0.28
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	6	0.28
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	14	0.28
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	14	0.28
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	10	0.28
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	13	0.28
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	10	0.28
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD11	9	0.28
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD12	9	0.28
(1,491)	1:40:B:VAL:HG21	1:126:B:LEU:HD13	9	0.28
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD11	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD12	9	0.28
(1,491)	1:40:B:VAL:HG22	1:126:B:LEU:HD13	9	0.28
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD11	9	0.28
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD12	9	0.28
(1,491)	1:40:B:VAL:HG23	1:126:B:LEU:HD13	9	0.28
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG11	18	0.28
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG12	18	0.28
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG13	18	0.28
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG11	18	0.28
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG12	18	0.28
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG13	18	0.28
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG11	18	0.28
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG12	18	0.28
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG13	18	0.28
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	14	0.28
(1,416)	1:14:B:GLN:H	1:84:B:PHE:HD1	6	0.28
(1,416)	1:14:B:GLN:H	1:84:B:PHE:HD2	6	0.28
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	6	0.28
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	3	0.28
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	3	0.28
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	17	0.28
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	10	0.28
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	11	0.28
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	7	0.28
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	7	0.28
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	7	0.28
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	20	0.28
(1,39)	1:19:A:LYS:H	1:79:A:GLN:H	8	0.28
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	17	0.28
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	20	0.28
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	6	0.28
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE1	17	0.27
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE2	17	0.27
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE3	17	0.27
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE1	17	0.27
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE2	17	0.27
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE3	17	0.27
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE1	17	0.27
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE2	17	0.27
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE3	17	0.27
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG11	9	0.27
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG12	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG13	9	0.27
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG11	9	0.27
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG12	9	0.27
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG13	9	0.27
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG11	9	0.27
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG12	9	0.27
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG13	9	0.27
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	16	0.27
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	16	0.27
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	16	0.27
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	18	0.27
(1,1495)	1:100:D:ALA:H	1:102:D:CYS:H	16	0.27
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB1	20	0.27
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB2	20	0.27
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB3	20	0.27
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD21	18	0.27
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD22	18	0.27
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD23	18	0.27
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD21	18	0.27
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD22	18	0.27
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD23	18	0.27
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	7	0.27
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	7	0.27
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	7	0.27
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	16	0.27
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	6	0.27
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	13	0.27
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	8	0.27
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	8	0.27
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	8	0.27
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	8	0.27
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	8	0.27
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	8	0.27
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	8	0.27
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	8	0.27
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	8	0.27
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	8	0.27
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	8	0.27
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	16	0.27
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	16	0.27
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	17	0.27
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	13	0.27
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	2	0.27
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	11	0.27
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	9	0.27
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	3	0.27
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	20	0.27
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	11	0.27
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	9	0.27
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	11	0.27
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	18	0.27
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	2	0.27
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	17	0.27
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	15	0.27
(1,1009)	1:64:C:VAL:HG11	1:126:C:LEU:HD21	12	0.27
(1,1009)	1:64:C:VAL:HG11	1:126:C:LEU:HD22	12	0.27
(1,1009)	1:64:C:VAL:HG11	1:126:C:LEU:HD23	12	0.27
(1,1009)	1:64:C:VAL:HG12	1:126:C:LEU:HD21	12	0.27
(1,1009)	1:64:C:VAL:HG12	1:126:C:LEU:HD22	12	0.27
(1,1009)	1:64:C:VAL:HG12	1:126:C:LEU:HD23	12	0.27
(1,1009)	1:64:C:VAL:HG13	1:126:C:LEU:HD21	12	0.27
(1,1009)	1:64:C:VAL:HG13	1:126:C:LEU:HD22	12	0.27
(1,1009)	1:64:C:VAL:HG13	1:126:C:LEU:HD23	12	0.27
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	16	0.27
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	18	0.27
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	18	0.27
(1,934)	1:49:C:SER:H	1:57:C:GLU:H	19	0.27
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	19	0.27
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	6	0.27
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD11	1	0.27
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD12	1	0.27
(1,894)	1:40:C:VAL:HG21	1:42:C:LEU:HD13	1	0.27
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD11	1	0.27
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD12	1	0.27
(1,894)	1:40:C:VAL:HG22	1:42:C:LEU:HD13	1	0.27
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD11	1	0.27
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD12	1	0.27
(1,894)	1:40:C:VAL:HG23	1:42:C:LEU:HD13	1	0.27
(1,866)	1:30:C:HIS:H	1:32:C:PHE:H	11	0.27
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	10	0.27
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	3	0.27
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	6	0.27
(1,790)	1:9:C:MET:H	1:10:C:THR:H	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	1	0.27
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	19	0.27
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	14	0.27
(1,679)	1:92:B:THR:H	1:94:B:MET:H	8	0.27
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	8	0.27
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	16	0.27
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	2	0.27
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD21	10	0.27
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD22	10	0.27
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD23	10	0.27
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD21	10	0.27
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD22	10	0.27
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD23	10	0.27
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	14	0.27
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	14	0.27
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	14	0.27
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD1	3	0.27
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD2	3	0.27
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	2	0.27
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	6	0.27
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE1	10	0.27
(1,519)	1:45:B:ASP:H	1:133:B:PHE:HE2	10	0.27
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	12	0.27
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	11	0.27
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	11	0.27
(1,335)	1:114:A:ILE:H	1:117:A:MET:H	19	0.27
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	19	0.27
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	1	0.27
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	11	0.27
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	16	0.27
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	8	0.27
(1,289)	1:95:A:ALA:H	1:98:A:LEU:H	13	0.27
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	1	0.27
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	10	0.27
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	18	0.27
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	18	0.27
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	18	0.27
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	17	0.27
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD21	17	0.27
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD22	17	0.27
(1,195)	1:62:A:VAL:HG11	1:128:A:LEU:HD23	17	0.27
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD21	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD22	17	0.27
(1,195)	1:62:A:VAL:HG12	1:128:A:LEU:HD23	17	0.27
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD21	17	0.27
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD22	17	0.27
(1,195)	1:62:A:VAL:HG13	1:128:A:LEU:HD23	17	0.27
(1,176)	1:59:A:VAL:HG11	1:80:A:GLN:H	12	0.27
(1,176)	1:59:A:VAL:HG12	1:80:A:GLN:H	12	0.27
(1,176)	1:59:A:VAL:HG13	1:80:A:GLN:H	12	0.27
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	16	0.27
(1,66)	1:28:A:ALA:H	1:30:A:HIS:H	10	0.27
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE1	5	0.27
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE2	5	0.27
(1,55)	1:23:A:PHE:HD1	1:117:A:MET:HE3	5	0.27
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE1	5	0.27
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE2	5	0.27
(1,55)	1:23:A:PHE:HD2	1:117:A:MET:HE3	5	0.27
(1,39)	1:19:A:LYS:H	1:79:A:GLN:H	9	0.27
(1,13)	1:11:A:PHE:HE1	1:102:A:CYS:H	5	0.27
(1,13)	1:11:A:PHE:HE2	1:102:A:CYS:H	5	0.27
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	17	0.26
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	17	0.26
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	17	0.26
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	12	0.26
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	12	0.26
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	12	0.26
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	12	0.26
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	12	0.26
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	12	0.26
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG11	16	0.26
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG12	16	0.26
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG13	16	0.26
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG11	16	0.26
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG12	16	0.26
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG13	16	0.26
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG11	16	0.26
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG12	16	0.26
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG13	16	0.26
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	13	0.26
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	13	0.26
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	13	0.26
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB1	8	0.26
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB2	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB3	8	0.26
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB1	8	0.26
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB2	8	0.26
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB3	8	0.26
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB1	8	0.26
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB2	8	0.26
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB3	8	0.26
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB1	8	0.26
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB2	8	0.26
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB3	8	0.26
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB1	8	0.26
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB2	8	0.26
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB3	8	0.26
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB1	8	0.26
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB2	8	0.26
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB3	8	0.26
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	3	0.26
(1,1334)	1:51:D:LEU:H	1:57:D:GLU:H	19	0.26
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	8	0.26
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	11	0.26
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	11	0.26
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	11	0.26
(1,1317)	1:47:D:ALA:H	1:61:D:ARG:H	11	0.26
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	14	0.26
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	7	0.26
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	16	0.26
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	1	0.26
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	17	0.26
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	14	0.26
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	10	0.26
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	3	0.26
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	3	0.26
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	3	0.26
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	17	0.26
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	1	0.26
(1,1108)	1:98:C:LEU:H	1:102:C:CYS:H	1	0.26
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	10	0.26
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	4	0.26
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	14	0.26
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	19	0.26
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	2	0.26
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	2	0.26
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	2	0.26
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	2	0.26
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	2	0.26
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	2	0.26
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	2	0.26
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	2	0.26
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	15	0.26
(1,908)	1:43:C:ASP:H	1:63:C:THR:H	5	0.26
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	16	0.26
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	16	0.26
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	16	0.26
(1,888)	1:39:C:GLU:H	1:67:C:SER:H	4	0.26
(1,885)	1:36:C:TRP:H	1:37:C:GLN:H	17	0.26
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	3	0.26
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	9	0.26
(1,753)	1:125:B:GLN:H	1:125:C:GLN:H	11	0.26
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	9	0.26
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	13	0.26
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	17	0.26
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	10	0.26
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	19	0.26
(1,595)	1:64:B:VAL:H	1:76:B:CYS:H	19	0.26
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	3	0.26
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	12	0.26
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	14	0.26
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	3	0.26
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	7	0.26
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	7	0.26
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	7	0.26
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	7	0.26
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	7	0.26
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	7	0.26
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	7	0.26
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	7	0.26
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	7	0.26
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	3	0.26
(1,382)	1:136:A:LEU:H	1:138:A:MET:H	17	0.26
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	11	0.26
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	3	0.26
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	11	0.26
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	8	0.26
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	15	0.26
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	12	0.26
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	17	0.26
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	15	0.26
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	15	0.26
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	15	0.26
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	1	0.26
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	8	0.26
(1,180)	1:59:A:VAL:HG21	1:82:A:GLY:H	9	0.26
(1,180)	1:59:A:VAL:HG22	1:82:A:GLY:H	9	0.26
(1,180)	1:59:A:VAL:HG23	1:82:A:GLY:H	9	0.26
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	11	0.26
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	11	0.26
(1,131)	1:47:A:ALA:H	1:61:A:ARG:H	15	0.26
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD21	1	0.26
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD22	1	0.26
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD23	1	0.26
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	4	0.26
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	4	0.26
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	4	0.26
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB1	1	0.26
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB2	1	0.26
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB3	1	0.26
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB1	1	0.26
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB2	1	0.26
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB3	1	0.26
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB1	1	0.26
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB2	1	0.26
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB3	1	0.26
(1,18)	1:14:A:GLN:H	1:83:A:ILE:H	18	0.26
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	5	0.26
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	6	0.25
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	6	0.25
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	6	0.25
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	6	0.25
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	6	0.25
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	6	0.25
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	19	0.25
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	19	0.25
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	19	0.25
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	19	0.25
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	19	0.25
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD11	7	0.25
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD12	7	0.25
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD13	7	0.25
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	4	0.25
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	4	0.25
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	4	0.25
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	4	0.25
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	4	0.25
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	4	0.25
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	12	0.25
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	12	0.25
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	12	0.25
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	12	0.25
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	12	0.25
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	12	0.25
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	13	0.25
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	13	0.25
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	13	0.25
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	13	0.25
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	13	0.25
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	13	0.25
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	15	0.25
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	15	0.25
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	15	0.25
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	15	0.25
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	15	0.25
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	15	0.25
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	15	0.25
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	15	0.25
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	15	0.25
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	6	0.25
(1,1472)	1:94:D:MET:H	1:96:D:HIS:H	4	0.25
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	17	0.25
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	18	0.25
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	5	0.25
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	17	0.25
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	20	0.25
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	1	0.25
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	18	0.25
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	19	0.25
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	6	0.25
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	20	0.25
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	2	0.25
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	9	0.25
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	12	0.25
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	10	0.25
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE1	9	0.25
(1,1048)	1:74:C:PHE:HE1	1:123:C:PHE:HE2	9	0.25
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE1	9	0.25
(1,1048)	1:74:C:PHE:HE2	1:123:C:PHE:HE2	9	0.25
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	16	0.25
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	13	0.25
(1,985)	1:60:C:LEU:H	1:81:C:GLY:H	14	0.25
(1,965)	1:56:C:TYR:H	1:84:C:PHE:H	15	0.25
(1,885)	1:36:C:TRP:H	1:37:C:GLN:H	3	0.25
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	11	0.25
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	1	0.25
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	5	0.25
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	1	0.25
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	2	0.25
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	8	0.25
(1,679)	1:92:B:THR:H	1:94:B:MET:H	13	0.25
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	3	0.25
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	12	0.25
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	12	0.25
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	12	0.25
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD21	13	0.25
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD22	13	0.25
(1,570)	1:58:B:VAL:HG21	1:98:B:LEU:HD23	13	0.25
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD21	13	0.25
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD22	13	0.25
(1,570)	1:58:B:VAL:HG22	1:98:B:LEU:HD23	13	0.25
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD21	13	0.25
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD22	13	0.25
(1,570)	1:58:B:VAL:HG23	1:98:B:LEU:HD23	13	0.25
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG21	20	0.25
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG22	20	0.25
(1,514)	1:44:B:LEU:HD21	1:131:B:VAL:HG23	20	0.25
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG21	20	0.25
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG22	20	0.25
(1,514)	1:44:B:LEU:HD22	1:131:B:VAL:HG23	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG21	20	0.25
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG22	20	0.25
(1,514)	1:44:B:LEU:HD23	1:131:B:VAL:HG23	20	0.25
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG11	6	0.25
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG12	6	0.25
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG13	6	0.25
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD11	7	0.25
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD12	7	0.25
(1,486)	1:40:B:VAL:HG11	1:128:B:LEU:HD13	7	0.25
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD11	7	0.25
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD12	7	0.25
(1,486)	1:40:B:VAL:HG12	1:128:B:LEU:HD13	7	0.25
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD11	7	0.25
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD12	7	0.25
(1,486)	1:40:B:VAL:HG13	1:128:B:LEU:HD13	7	0.25
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	19	0.25
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	19	0.25
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	19	0.25
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	19	0.25
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	19	0.25
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	19	0.25
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	19	0.25
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	19	0.25
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	19	0.25
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	4	0.25
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	12	0.25
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	7	0.25
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	20	0.25
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	13	0.25
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	11	0.25
(1,221)	1:67:A:SER:H	1:73:A:ALA:H	19	0.25
(1,180)	1:59:A:VAL:HG21	1:82:A:GLY:H	6	0.25
(1,180)	1:59:A:VAL:HG22	1:82:A:GLY:H	6	0.25
(1,180)	1:59:A:VAL:HG23	1:82:A:GLY:H	6	0.25
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	1	0.25
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	1	0.25
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	4	0.25
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	3	0.25
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	3	0.25
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	4	0.25
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	8	0.25
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	4	0.25
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	4	0.25
(1,66)	1:28:A:ALA:H	1:30:A:HIS:H	13	0.25
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	12	0.25
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	8	0.24
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	8	0.24
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	8	0.24
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	8	0.24
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	8	0.24
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	8	0.24
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD11	19	0.24
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD12	19	0.24
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD13	19	0.24
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	4	0.24
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	4	0.24
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	4	0.24
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	4	0.24
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	4	0.24
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	4	0.24
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG11	12	0.24
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG12	12	0.24
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG13	12	0.24
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG11	12	0.24
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG12	12	0.24
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG13	12	0.24
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG11	12	0.24
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG12	12	0.24
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG13	12	0.24
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	7	0.24
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	7	0.24
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	7	0.24
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	6	0.24
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	6	0.24
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	6	0.24
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	20	0.24
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	20	0.24
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	20	0.24
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	1	0.24
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	1	0.24
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	1	0.24
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	1	0.24
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	1	0.24
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	1	0.24
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	1	0.24
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	1	0.24
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	1	0.24
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	1	0.24
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	1	0.24
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	1	0.24
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	1	0.24
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	1	0.24
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	1	0.24
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	1	0.24
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	1	0.24
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	1	0.24
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	1	0.24
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	1	0.24
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	1	0.24
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	1	0.24
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	1	0.24
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	1	0.24
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	1	0.24
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	1	0.24
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	1	0.24
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	1	0.24
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	1	0.24
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	1	0.24
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	1	0.24
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	1	0.24
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	1	0.24
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	1	0.24
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	1	0.24
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD1	9	0.24
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD2	9	0.24
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD1	9	0.24
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD2	9	0.24
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD1	9	0.24
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD2	9	0.24
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	12	0.24
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	12	0.24
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	12	0.24
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	12	0.24
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	12	0.24
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	14	0.24
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	14	0.24
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	14	0.24
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	14	0.24
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	14	0.24
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	14	0.24
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	18	0.24
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	18	0.24
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	18	0.24
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	18	0.24
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	18	0.24
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	18	0.24
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	6	0.24
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	14	0.24
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	14	0.24
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	14	0.24
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	14	0.24
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	14	0.24
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	14	0.24
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	14	0.24
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	14	0.24
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	14	0.24
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	5	0.24
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	7	0.24
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	13	0.24
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	3	0.24
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB1	8	0.24
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB2	8	0.24
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB3	8	0.24
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	10	0.24
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	19	0.24
(1,1334)	1:51:D:LEU:H	1:57:D:GLU:H	14	0.24
(1,1334)	1:51:D:LEU:H	1:57:D:GLU:H	20	0.24
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD21	15	0.24
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD22	15	0.24
(1,1327)	1:49:D:SER:H	1:98:D:LEU:HD23	15	0.24
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG11	12	0.24
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG12	12	0.24
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG13	12	0.24
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	10	0.24
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	9	0.24
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	13	0.24
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	8	0.24
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	8	0.24
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	15	0.24
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	16	0.24
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	2	0.24
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	15	0.24
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	4	0.24
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	11	0.24
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	7	0.24
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD11	12	0.24
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD12	12	0.24
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD13	12	0.24
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD11	12	0.24
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD12	12	0.24
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD13	12	0.24
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD11	12	0.24
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD12	12	0.24
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD13	12	0.24
(1,984)	1:60:C:LEU:H	1:80:C:GLN:H	5	0.24
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	17	0.24
(1,965)	1:56:C:TYR:H	1:84:C:PHE:H	13	0.24
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	1	0.24
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	17	0.24
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	19	0.24
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	17	0.24
(1,934)	1:49:C:SER:H	1:57:C:GLU:H	16	0.24
(1,927)	1:47:C:ALA:H	1:60:C:LEU:H	8	0.24
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD11	19	0.24
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD12	19	0.24
(1,916)	1:44:C:LEU:HD21	1:128:C:LEU:HD13	19	0.24
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD11	19	0.24
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD12	19	0.24
(1,916)	1:44:C:LEU:HD22	1:128:C:LEU:HD13	19	0.24
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD11	19	0.24
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD12	19	0.24
(1,916)	1:44:C:LEU:HD23	1:128:C:LEU:HD13	19	0.24
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	14	0.24
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	12	0.24
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	12	0.24
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	16	0.24
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	16	0.24
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	16	0.24
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	8	0.24
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	13	0.24
(1,800)	1:11:C:PHE:HE1	1:12:C:GLN:H	5	0.24
(1,800)	1:11:C:PHE:HE2	1:12:C:GLN:H	5	0.24
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	20	0.24
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	7	0.24
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	10	0.24
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	14	0.24
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	14	0.24
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	14	0.24
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	14	0.24
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	14	0.24
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	14	0.24
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	14	0.24
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	14	0.24
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	14	0.24
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD21	20	0.24
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD22	20	0.24
(1,755)	1:126:B:LEU:HD11	1:128:B:LEU:HD23	20	0.24
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD21	20	0.24
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD22	20	0.24
(1,755)	1:126:B:LEU:HD12	1:128:B:LEU:HD23	20	0.24
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD21	20	0.24
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD22	20	0.24
(1,755)	1:126:B:LEU:HD13	1:128:B:LEU:HD23	20	0.24
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	15	0.24
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	19	0.24
(1,679)	1:92:B:THR:H	1:94:B:MET:H	3	0.24
(1,679)	1:92:B:THR:H	1:94:B:MET:H	6	0.24
(1,679)	1:92:B:THR:H	1:94:B:MET:H	15	0.24
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	18	0.24
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	20	0.24
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	17	0.24
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	4	0.24
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	17	0.24
(1,595)	1:64:B:VAL:H	1:76:B:CYS:H	9	0.24
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	6	0.24
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	11	0.24
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	18	0.24
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	19	0.24
(1,569)	1:58:B:VAL:HG21	1:98:B:LEU:HD11	13	0.24
(1,569)	1:58:B:VAL:HG21	1:98:B:LEU:HD12	13	0.24
(1,569)	1:58:B:VAL:HG21	1:98:B:LEU:HD13	13	0.24
(1,569)	1:58:B:VAL:HG22	1:98:B:LEU:HD11	13	0.24
(1,569)	1:58:B:VAL:HG22	1:98:B:LEU:HD12	13	0.24
(1,569)	1:58:B:VAL:HG22	1:98:B:LEU:HD13	13	0.24
(1,569)	1:58:B:VAL:HG23	1:98:B:LEU:HD11	13	0.24
(1,569)	1:58:B:VAL:HG23	1:98:B:LEU:HD12	13	0.24
(1,569)	1:58:B:VAL:HG23	1:98:B:LEU:HD13	13	0.24
(1,560)	1:57:B:GLU:H	1:58:B:VAL:H	2	0.24
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	5	0.24
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	11	0.24
(1,532)	1:49:B:SER:H	1:59:B:VAL:H	5	0.24
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	15	0.24
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	11	0.24
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	11	0.24
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	11	0.24
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	11	0.24
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	11	0.24
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	11	0.24
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	11	0.24
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	11	0.24
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	11	0.24
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	3	0.24
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	2	0.24
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	6	0.24
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	9	0.24
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	14	0.24
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	8	0.24
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	10	0.24
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	11	0.24
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	5	0.24
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	20	0.24
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	17	0.24
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	14	0.24
(1,212)	1:66:A:ALA:H	1:74:A:PHE:HE1	11	0.24
(1,212)	1:66:A:ALA:H	1:74:A:PHE:HE2	11	0.24
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	2	0.24
(1,177)	1:59:A:VAL:HG11	1:81:A:GLY:H	13	0.24
(1,177)	1:59:A:VAL:HG12	1:81:A:GLY:H	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:59:A:VAL:HG13	1:81:A:GLY:H	13	0.24
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	3	0.24
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	7	0.24
(1,103)	1:41:A:LYS:H	1:65:A:THR:H	6	0.24
(1,5)	1:11:A:PHE:HD1	1:12:A:GLN:H	4	0.24
(1,5)	1:11:A:PHE:HD2	1:12:A:GLN:H	4	0.24
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD11	2	0.23
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD12	2	0.23
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD13	2	0.23
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD11	12	0.23
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD12	12	0.23
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD13	12	0.23
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	13	0.23
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	13	0.23
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	13	0.23
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	13	0.23
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	13	0.23
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	13	0.23
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD11	3	0.23
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD12	3	0.23
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD13	3	0.23
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE1	17	0.23
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE2	17	0.23
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE1	17	0.23
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE2	17	0.23
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE1	17	0.23
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE2	17	0.23
(1,1639)	1:36:C:TRP:HZ2	2:470:G:LEU:HD11	3	0.23
(1,1639)	1:36:C:TRP:HZ2	2:470:G:LEU:HD12	3	0.23
(1,1639)	1:36:C:TRP:HZ2	2:470:G:LEU:HD13	3	0.23
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD11	3	0.23
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD12	3	0.23
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD13	3	0.23
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD21	3	0.23
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD22	3	0.23
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD23	3	0.23
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD11	3	0.23
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD12	3	0.23
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD13	3	0.23
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD21	3	0.23
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD22	3	0.23
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD23	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD11	3	0.23
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD12	3	0.23
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD13	3	0.23
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD21	3	0.23
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD22	3	0.23
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD23	3	0.23
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD11	3	0.23
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD12	3	0.23
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD13	3	0.23
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD21	3	0.23
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD22	3	0.23
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD23	3	0.23
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD11	3	0.23
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD12	3	0.23
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD13	3	0.23
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD21	3	0.23
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD22	3	0.23
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD23	3	0.23
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD11	3	0.23
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD12	3	0.23
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD13	3	0.23
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD21	3	0.23
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD22	3	0.23
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD23	3	0.23
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE1	2	0.23
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE2	2	0.23
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE3	2	0.23
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE1	2	0.23
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE2	2	0.23
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE3	2	0.23
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE1	2	0.23
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE2	2	0.23
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE3	2	0.23
(1,1624)	1:133:B:PHE:HD1	2:460:F:LEU:HD11	14	0.23
(1,1624)	1:133:B:PHE:HD1	2:460:F:LEU:HD12	14	0.23
(1,1624)	1:133:B:PHE:HD1	2:460:F:LEU:HD13	14	0.23
(1,1624)	1:133:B:PHE:HD2	2:460:F:LEU:HD11	14	0.23
(1,1624)	1:133:B:PHE:HD2	2:460:F:LEU:HD12	14	0.23
(1,1624)	1:133:B:PHE:HD2	2:460:F:LEU:HD13	14	0.23
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD11	6	0.23
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD12	6	0.23
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD13	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD11	13	0.23
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD12	13	0.23
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD13	13	0.23
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG11	14	0.23
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG12	14	0.23
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG13	14	0.23
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG21	14	0.23
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG22	14	0.23
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG23	14	0.23
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG11	14	0.23
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG12	14	0.23
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG13	14	0.23
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG21	14	0.23
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG22	14	0.23
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG23	14	0.23
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG11	14	0.23
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG12	14	0.23
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG13	14	0.23
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG21	14	0.23
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG22	14	0.23
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG23	14	0.23
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	3	0.23
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	4	0.23
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	20	0.23
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	19	0.23
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	12	0.23
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB1	19	0.23
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB2	19	0.23
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB3	19	0.23
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	12	0.23
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	12	0.23
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	12	0.23
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	14	0.23
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	14	0.23
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	14	0.23
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD11	3	0.23
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD12	3	0.23
(1,1355)	1:56:D:TYR:HE1	1:98:D:LEU:HD13	3	0.23
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD11	3	0.23
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD12	3	0.23
(1,1355)	1:56:D:TYR:HE2	1:98:D:LEU:HD13	3	0.23
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	11	0.23
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	6	0.23
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD21	12	0.23
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD22	12	0.23
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD23	12	0.23
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD21	12	0.23
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD22	12	0.23
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD23	12	0.23
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD21	12	0.23
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD22	12	0.23
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD23	12	0.23
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	12	0.23
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	10	0.23
(1,1264)	1:31:D:VAL:HG21	1:68:D:LEU:HD11	2	0.23
(1,1264)	1:31:D:VAL:HG21	1:68:D:LEU:HD12	2	0.23
(1,1264)	1:31:D:VAL:HG21	1:68:D:LEU:HD13	2	0.23
(1,1264)	1:31:D:VAL:HG22	1:68:D:LEU:HD11	2	0.23
(1,1264)	1:31:D:VAL:HG22	1:68:D:LEU:HD12	2	0.23
(1,1264)	1:31:D:VAL:HG22	1:68:D:LEU:HD13	2	0.23
(1,1264)	1:31:D:VAL:HG23	1:68:D:LEU:HD11	2	0.23
(1,1264)	1:31:D:VAL:HG23	1:68:D:LEU:HD12	2	0.23
(1,1264)	1:31:D:VAL:HG23	1:68:D:LEU:HD13	2	0.23
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	11	0.23
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	11	0.23
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	2	0.23
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	9	0.23
(1,1194)	1:138:C:MET:H	1:140:C:TYR:H	6	0.23
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	10	0.23
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	1	0.23
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	6	0.23
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	6	0.23
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	6	0.23
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	6	0.23
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	6	0.23
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	6	0.23
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	6	0.23
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	6	0.23
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	6	0.23
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	14	0.23
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	16	0.23
(1,1126)	1:110:C:ALA:H	1:112:C:GLU:H	14	0.23
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	12	0.23
(1,1079)	1:90:C:GLU:H	1:93:C:GLN:H	17	0.23
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	9	0.23
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	17	0.23
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	10	0.23
(1,944)	1:51:C:LEU:H	1:56:C:TYR:H	1	0.23
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	10	0.23
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	8	0.23
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	16	0.23
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	18	0.23
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	15	0.23
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	15	0.23
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	15	0.23
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	13	0.23
(1,899)	1:41:C:LYS:H	1:67:C:SER:H	19	0.23
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	17	0.23
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	17	0.23
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	17	0.23
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	15	0.23
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	7	0.23
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	5	0.23
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	19	0.23
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	13	0.23
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	20	0.23
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	18	0.23
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	9	0.23
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	9	0.23
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	9	0.23
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	9	0.23
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	9	0.23
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	9	0.23
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	9	0.23
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	9	0.23
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	9	0.23
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	16	0.23
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	9	0.23
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	2	0.23
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	14	0.23
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	20	0.23
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	4	0.23
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	17	0.23
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	3	0.23
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	6	0.23
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	10	0.23
(1,560)	1:57:B:GLU:H	1:58:B:VAL:H	11	0.23
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	18	0.23
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	12	0.23
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	11	0.23
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	7	0.23
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	11	0.23
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	14	0.23
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	14	0.23
(1,354)	1:119:A:SER:H	1:123:A:PHE:H	14	0.23
(1,335)	1:114:A:ILE:H	1:117:A:MET:H	15	0.23
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	6	0.23
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	12	0.23
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	8	0.23
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	16	0.23
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	12	0.23
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	17	0.23
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	5	0.23
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	9	0.23
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG21	4	0.23
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG22	4	0.23
(1,193)	1:62:A:VAL:HG11	1:64:A:VAL:HG23	4	0.23
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG21	4	0.23
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG22	4	0.23
(1,193)	1:62:A:VAL:HG12	1:64:A:VAL:HG23	4	0.23
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG21	4	0.23
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG22	4	0.23
(1,193)	1:62:A:VAL:HG13	1:64:A:VAL:HG23	4	0.23
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	12	0.23
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	15	0.23
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	1	0.23
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	14	0.23
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	14	0.23
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	14	0.23
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG21	4	0.23
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG22	4	0.23
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG23	4	0.23
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG21	4	0.23
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG22	4	0.23
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG23	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG21	4	0.23
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG22	4	0.23
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG23	4	0.23
(1,103)	1:41:A:LYS:H	1:65:A:THR:H	7	0.23
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	15	0.23
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	6	0.23
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB1	12	0.23
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB2	12	0.23
(1,64)	1:25:A:ALA:HB1	1:28:A:ALA:HB3	12	0.23
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB1	12	0.23
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB2	12	0.23
(1,64)	1:25:A:ALA:HB2	1:28:A:ALA:HB3	12	0.23
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB1	12	0.23
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB2	12	0.23
(1,64)	1:25:A:ALA:HB3	1:28:A:ALA:HB3	12	0.23
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE1	5	0.23
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE2	5	0.23
(1,52)	1:23:A:PHE:H	1:117:A:MET:HE3	5	0.23
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG11	14	0.22
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG12	14	0.22
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG13	14	0.22
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG11	14	0.22
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG12	14	0.22
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG13	14	0.22
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG11	14	0.22
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG12	14	0.22
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG13	14	0.22
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD11	15	0.22
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD12	15	0.22
(1,1667)	1:36:D:TRP:HE1	2:470:H:LEU:HD13	15	0.22
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD11	3	0.22
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD12	3	0.22
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD13	3	0.22
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD21	3	0.22
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD22	3	0.22
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD23	3	0.22
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD11	3	0.22
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD12	3	0.22
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD13	3	0.22
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD21	3	0.22
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD22	3	0.22
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD23	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD11	3	0.22
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD12	3	0.22
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD13	3	0.22
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD21	3	0.22
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD22	3	0.22
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD23	3	0.22
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD11	3	0.22
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD12	3	0.22
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD13	3	0.22
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD21	3	0.22
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD22	3	0.22
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD23	3	0.22
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD11	3	0.22
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD12	3	0.22
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD13	3	0.22
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD21	3	0.22
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD22	3	0.22
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD23	3	0.22
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD11	3	0.22
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD12	3	0.22
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD13	3	0.22
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD21	3	0.22
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD22	3	0.22
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD23	3	0.22
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD21	8	0.22
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD22	8	0.22
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD23	8	0.22
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD21	8	0.22
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD22	8	0.22
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD23	8	0.22
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD21	8	0.22
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD22	8	0.22
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD23	8	0.22
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	17	0.22
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	17	0.22
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	17	0.22
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	17	0.22
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	17	0.22
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	17	0.22
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG11	18	0.22
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG12	18	0.22
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG13	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG11	18	0.22
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG12	18	0.22
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG13	18	0.22
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG11	18	0.22
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG12	18	0.22
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG13	18	0.22
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	5	0.22
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	14	0.22
(1,1495)	1:100:D:ALA:H	1:102:D:CYS:H	15	0.22
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	10	0.22
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	8	0.22
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	20	0.22
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD21	10	0.22
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD22	10	0.22
(1,1429)	1:74:D:PHE:H	1:75:D:LEU:HD23	10	0.22
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	3	0.22
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD21	7	0.22
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD22	7	0.22
(1,1363)	1:58:D:VAL:HG21	1:98:D:LEU:HD23	7	0.22
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD21	7	0.22
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD22	7	0.22
(1,1363)	1:58:D:VAL:HG22	1:98:D:LEU:HD23	7	0.22
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD21	7	0.22
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD22	7	0.22
(1,1363)	1:58:D:VAL:HG23	1:98:D:LEU:HD23	7	0.22
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	17	0.22
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	12	0.22
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	15	0.22
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	12	0.22
(1,1313)	1:46:D:THR:H	1:61:D:ARG:H	11	0.22
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD21	18	0.22
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD22	18	0.22
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD23	18	0.22
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD21	18	0.22
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD22	18	0.22
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD23	18	0.22
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD21	18	0.22
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD22	18	0.22
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD23	18	0.22
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD11	7	0.22
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD12	7	0.22
(1,1288)	1:40:D:VAL:HG21	1:126:D:LEU:HD13	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD11	7	0.22
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD12	7	0.22
(1,1288)	1:40:D:VAL:HG22	1:126:D:LEU:HD13	7	0.22
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD11	7	0.22
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD12	7	0.22
(1,1288)	1:40:D:VAL:HG23	1:126:D:LEU:HD13	7	0.22
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	11	0.22
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	18	0.22
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	19	0.22
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	4	0.22
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	4	0.22
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	6	0.22
(1,1225)	1:19:D:LYS:H	1:79:D:GLN:H	10	0.22
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	1	0.22
(1,1189)	1:137:C:PHE:H	1:140:C:TYR:H	17	0.22
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	3	0.22
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	1	0.22
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	8	0.22
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	15	0.22
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	18	0.22
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	13	0.22
(1,949)	1:51:C:LEU:HD21	1:57:C:GLU:H	1	0.22
(1,949)	1:51:C:LEU:HD22	1:57:C:GLU:H	1	0.22
(1,949)	1:51:C:LEU:HD23	1:57:C:GLU:H	1	0.22
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	4	0.22
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	14	0.22
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	14	0.22
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	14	0.22
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	6	0.22
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	11	0.22
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	11	0.22
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	9	0.22
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	10	0.22
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	1	0.22
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	5	0.22
(1,708)	1:100:B:ALA:H	1:101:B:TYR:H	8	0.22
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	2	0.22
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	18	0.22
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	11	0.22
(1,699)	1:97:B:CYS:H	1:101:B:TYR:H	16	0.22
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	6	0.22
(1,679)	1:92:B:THR:H	1:94:B:MET:H	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	9	0.22
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	9	0.22
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	9	0.22
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	14	0.22
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	14	0.22
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	14	0.22
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	13	0.22
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	3	0.22
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	12	0.22
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD1	16	0.22
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD2	16	0.22
(1,528)	1:48:B:SER:H	1:59:B:VAL:H	19	0.22
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	8	0.22
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	7	0.22
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	7	0.22
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	12	0.22
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	12	0.22
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	4	0.22
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	4	0.22
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	7	0.22
(1,345)	1:117:A:MET:HE1	1:117:B:MET:HE1	6	0.22
(1,345)	1:117:A:MET:HE1	1:117:B:MET:HE2	6	0.22
(1,345)	1:117:A:MET:HE1	1:117:B:MET:HE3	6	0.22
(1,345)	1:117:A:MET:HE2	1:117:B:MET:HE1	6	0.22
(1,345)	1:117:A:MET:HE2	1:117:B:MET:HE2	6	0.22
(1,345)	1:117:A:MET:HE2	1:117:B:MET:HE3	6	0.22
(1,345)	1:117:A:MET:HE3	1:117:B:MET:HE1	6	0.22
(1,345)	1:117:A:MET:HE3	1:117:B:MET:HE2	6	0.22
(1,345)	1:117:A:MET:HE3	1:117:B:MET:HE3	6	0.22
(1,335)	1:114:A:ILE:H	1:117:A:MET:H	10	0.22
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	8	0.22
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	11	0.22
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	5	0.22
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	8	0.22
(1,221)	1:67:A:SER:H	1:73:A:ALA:H	17	0.22
(1,180)	1:59:A:VAL:HG21	1:82:A:GLY:H	20	0.22
(1,180)	1:59:A:VAL:HG22	1:82:A:GLY:H	20	0.22
(1,180)	1:59:A:VAL:HG23	1:82:A:GLY:H	20	0.22
(1,176)	1:59:A:VAL:HG11	1:80:A:GLN:H	6	0.22
(1,176)	1:59:A:VAL:HG12	1:80:A:GLN:H	6	0.22
(1,176)	1:59:A:VAL:HG13	1:80:A:GLN:H	6	0.22
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	2	0.22
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	2	0.22
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD1	11	0.22
(1,159)	1:55:A:VAL:H	1:56:A:TYR:HD2	11	0.22
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	1	0.22
(1,115)	1:43:A:ASP:H	1:63:A:THR:H	2	0.22
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	4	0.22
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	11	0.21
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	11	0.21
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	11	0.21
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	11	0.21
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	11	0.21
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	11	0.21
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB1	4	0.21
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB2	4	0.21
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB3	4	0.21
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB1	4	0.21
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB2	4	0.21
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB3	4	0.21
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB1	4	0.21
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB2	4	0.21
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB3	4	0.21
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB1	4	0.21
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB2	4	0.21
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB3	4	0.21
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB1	4	0.21
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB2	4	0.21
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB3	4	0.21
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB1	4	0.21
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB2	4	0.21
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB3	4	0.21
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE1	12	0.21
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE2	12	0.21
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE3	12	0.21
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE1	12	0.21
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE2	12	0.21
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE3	12	0.21
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE1	12	0.21
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE2	12	0.21
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE3	12	0.21
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD11	10	0.21
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD12	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD13	10	0.21
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD11	10	0.21
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD12	10	0.21
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD13	10	0.21
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD11	10	0.21
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD12	10	0.21
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD13	10	0.21
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	7	0.21
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	7	0.21
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	7	0.21
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	7	0.21
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	7	0.21
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	7	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	13	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	13	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	13	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	13	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	13	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	13	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	14	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	14	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	14	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	14	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	14	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	14	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	18	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	18	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	18	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	18	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	18	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	18	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	19	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	19	0.21
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	19	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	19	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	19	0.21
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	19	0.21
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG11	6	0.21
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG12	6	0.21
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG13	6	0.21
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG21	6	0.21
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG22	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG23	6	0.21
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG11	6	0.21
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG12	6	0.21
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG13	6	0.21
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG21	6	0.21
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG22	6	0.21
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG23	6	0.21
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG11	6	0.21
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG12	6	0.21
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG13	6	0.21
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG21	6	0.21
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG22	6	0.21
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG23	6	0.21
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG21	4	0.21
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG22	4	0.21
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG23	4	0.21
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG21	4	0.21
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG22	4	0.21
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG23	4	0.21
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	20	0.21
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	5	0.21
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	5	0.21
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	5	0.21
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	5	0.21
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	5	0.21
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	5	0.21
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	5	0.21
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	5	0.21
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	5	0.21
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	2	0.21
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	2	0.21
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	2	0.21
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	2	0.21
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	2	0.21
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	2	0.21
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	2	0.21
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	2	0.21
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	2	0.21
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	6	0.21
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	6	0.21
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	6	0.21
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	6	0.21
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	6	0.21
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	6	0.21
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	6	0.21
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	6	0.21
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	16	0.21
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	4	0.21
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	4	0.21
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	4	0.21
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	4	0.21
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	4	0.21
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	4	0.21
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	4	0.21
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	4	0.21
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	4	0.21
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE1	15	0.21
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE2	15	0.21
(1,1352)	1:56:D:TYR:HD1	1:94:D:MET:HE3	15	0.21
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE1	15	0.21
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE2	15	0.21
(1,1352)	1:56:D:TYR:HD2	1:94:D:MET:HE3	15	0.21
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	1	0.21
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	12	0.21
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	14	0.21
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	7	0.21
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	9	0.21
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD21	7	0.21
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD22	7	0.21
(1,1305)	1:44:D:LEU:HD11	1:60:D:LEU:HD23	7	0.21
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD21	7	0.21
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD22	7	0.21
(1,1305)	1:44:D:LEU:HD12	1:60:D:LEU:HD23	7	0.21
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD21	7	0.21
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD22	7	0.21
(1,1305)	1:44:D:LEU:HD13	1:60:D:LEU:HD23	7	0.21
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	15	0.21
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	11	0.21
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	11	0.21
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	11	0.21
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	11	0.21
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	11	0.21
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	11	0.21
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	11	0.21
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	11	0.21
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	18	0.21
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	18	0.21
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	18	0.21
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	18	0.21
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	18	0.21
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	18	0.21
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	18	0.21
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	18	0.21
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	18	0.21
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	12	0.21
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	15	0.21
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	12	0.21
(1,1182)	1:135:C:ALA:H	1:138:C:MET:H	6	0.21
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG21	5	0.21
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG22	5	0.21
(1,1168)	1:128:C:LEU:HD21	1:131:C:VAL:HG23	5	0.21
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG21	5	0.21
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG22	5	0.21
(1,1168)	1:128:C:LEU:HD22	1:131:C:VAL:HG23	5	0.21
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG21	5	0.21
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG22	5	0.21
(1,1168)	1:128:C:LEU:HD23	1:131:C:VAL:HG23	5	0.21
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	2	0.21
(1,1157)	1:121:C:GLY:H	1:123:C:PHE:H	19	0.21
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	7	0.21
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	7	0.21
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	12	0.21
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	15	0.21
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	18	0.21
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	10	0.21
(1,1030)	1:68:C:LEU:H	1:73:C:ALA:H	4	0.21
(1,1029)	1:68:C:LEU:H	1:71:C:GLU:H	11	0.21
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	7	0.21
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	7	0.21
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	9	0.21
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	3	0.21
(1,921)	1:45:C:ASP:H	1:63:C:THR:H	7	0.21
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	3	0.21
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	3	0.21
(1,866)	1:30:C:HIS:H	1:32:C:PHE:H	16	0.21
(1,860)	1:28:C:ALA:H	1:30:C:HIS:H	18	0.21
(1,844)	1:22:C:SER:H	1:23:D:PHE:H	14	0.21
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	13	0.21
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	19	0.21
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	18	0.21
(1,697)	1:97:B:CYS:H	1:99:B:GLY:H	3	0.21
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	10	0.21
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	10	0.21
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	20	0.21
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	13	0.21
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	13	0.21
(1,623)	1:68:B:LEU:H	1:72:B:THR:H	12	0.21
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	9	0.21
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	20	0.21
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	12	0.21
(1,595)	1:64:B:VAL:H	1:76:B:CYS:H	11	0.21
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	2	0.21
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	19	0.21
(1,532)	1:49:B:SER:H	1:59:B:VAL:H	10	0.21
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	2	0.21
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG11	5	0.21
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG12	5	0.21
(1,483)	1:40:B:VAL:HG11	1:64:B:VAL:HG13	5	0.21
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG11	5	0.21
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG12	5	0.21
(1,483)	1:40:B:VAL:HG12	1:64:B:VAL:HG13	5	0.21
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG11	5	0.21
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG12	5	0.21
(1,483)	1:40:B:VAL:HG13	1:64:B:VAL:HG13	5	0.21
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	1	0.21
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	10	0.21
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	11	0.21
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	13	0.21
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	5	0.21
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	8	0.21
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	8	0.21
(1,359)	1:122:A:THR:H	1:18:B:THR:H	2	0.21
(1,354)	1:119:A:SER:H	1:123:A:PHE:H	8	0.21
(1,335)	1:114:A:ILE:H	1:117:A:MET:H	2	0.21
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	4	0.21
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	6	0.21
(1,266)	1:85:A:SER:H	1:86:A:ILE:H	20	0.21
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	9	0.21
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	7	0.21
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	13	0.21
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB1	14	0.21
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB2	14	0.21
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB3	14	0.21
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB1	14	0.21
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB2	14	0.21
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB3	14	0.21
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB1	14	0.21
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB2	14	0.21
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB3	14	0.21
(1,184)	1:60:A:LEU:HD11	1:61:A:ARG:H	14	0.21
(1,184)	1:60:A:LEU:HD12	1:61:A:ARG:H	14	0.21
(1,184)	1:60:A:LEU:HD13	1:61:A:ARG:H	14	0.21
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	10	0.21
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	9	0.21
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	8	0.21
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD11	15	0.21
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD12	15	0.21
(1,120)	1:44:A:LEU:HD11	1:60:A:LEU:HD13	15	0.21
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD11	15	0.21
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD12	15	0.21
(1,120)	1:44:A:LEU:HD12	1:60:A:LEU:HD13	15	0.21
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD11	15	0.21
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD12	15	0.21
(1,120)	1:44:A:LEU:HD13	1:60:A:LEU:HD13	15	0.21
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	1	0.21
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	1	0.21
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	1	0.21
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	8	0.21
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	8	0.21
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	8	0.21
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	20	0.21
(1,77)	1:31:A:VAL:HG21	1:36:A:TRP:HE3	14	0.21
(1,77)	1:31:A:VAL:HG22	1:36:A:TRP:HE3	14	0.21
(1,77)	1:31:A:VAL:HG23	1:36:A:TRP:HE3	14	0.21
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	13	0.21
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG11	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG12	7	0.2
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG13	7	0.2
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG11	7	0.2
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG12	7	0.2
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG13	7	0.2
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG11	7	0.2
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG12	7	0.2
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG13	7	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB1	15	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB2	15	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB3	15	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB1	15	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB2	15	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB3	15	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB1	15	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB2	15	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB3	15	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB1	15	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB2	15	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB3	15	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB1	15	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB2	15	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB3	15	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB1	15	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB2	15	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB3	15	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB1	20	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB2	20	0.2
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB3	20	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB1	20	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB2	20	0.2
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB3	20	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB1	20	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB2	20	0.2
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB3	20	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB1	20	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB2	20	0.2
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB3	20	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB1	20	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB2	20	0.2
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB3	20	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB1	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB2	20	0.2
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB3	20	0.2
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG11	18	0.2
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG12	18	0.2
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG13	18	0.2
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG11	18	0.2
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG12	18	0.2
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG13	18	0.2
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG11	18	0.2
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG12	18	0.2
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG13	18	0.2
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	12	0.2
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	12	0.2
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	12	0.2
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	6	0.2
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	6	0.2
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	6	0.2
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	6	0.2
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	6	0.2
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	6	0.2
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE1	1	0.2
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE2	1	0.2
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE1	1	0.2
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE2	1	0.2
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE1	1	0.2
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE2	1	0.2
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	3	0.2
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	3	0.2
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	3	0.2
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	3	0.2
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	3	0.2
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	3	0.2
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	11	0.2
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	11	0.2
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	11	0.2
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	11	0.2
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	11	0.2
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	11	0.2
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	2	0.2
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	2	0.2
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	2	0.2
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	2	0.2
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	2	0.2
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	8	0.2
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	12	0.2
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	18	0.2
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	16	0.2
(1,1490)	1:99:D:GLY:H	1:100:D:ALA:H	13	0.2
(1,1471)	1:94:D:MET:H	1:95:D:ALA:H	7	0.2
(1,1467)	1:92:D:THR:H	1:95:D:ALA:H	19	0.2
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	19	0.2
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	19	0.2
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	19	0.2
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	13	0.2
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	7	0.2
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD11	13	0.2
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD12	13	0.2
(1,1353)	1:56:D:TYR:HD1	1:98:D:LEU:HD13	13	0.2
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD11	13	0.2
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD12	13	0.2
(1,1353)	1:56:D:TYR:HD2	1:98:D:LEU:HD13	13	0.2
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	19	0.2
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	7	0.2
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	6	0.2
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	13	0.2
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG11	3	0.2
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG12	3	0.2
(1,1290)	1:41:D:LYS:H	1:64:D:VAL:HG13	3	0.2
(1,1282)	1:39:D:GLU:H	1:67:D:SER:H	14	0.2
(1,1271)	1:35:D:ASP:H	1:36:D:TRP:H	14	0.2
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	2	0.2
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	9	0.2
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	15	0.2
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	15	0.2
(1,1203)	1:11:D:PHE:HD1	1:12:D:GLN:H	19	0.2
(1,1203)	1:11:D:PHE:HD2	1:12:D:GLN:H	19	0.2
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	2	0.2
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	11	0.2
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	4	0.2
(1,1099)	1:96:C:HIS:H	1:99:C:GLY:H	16	0.2
(1,1094)	1:95:C:ALA:H	1:98:C:LEU:H	9	0.2
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	13	0.2
(1,1055)	1:77:C:GLU:H	1:78:C:VAL:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:77:C:GLU:H	1:78:C:VAL:H	17	0.2
(1,1030)	1:68:C:LEU:H	1:73:C:ALA:H	17	0.2
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	11	0.2
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	18	0.2
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	18	0.2
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	18	0.2
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	18	0.2
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	18	0.2
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	18	0.2
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	18	0.2
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	18	0.2
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	18	0.2
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	12	0.2
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	15	0.2
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	19	0.2
(1,941)	1:51:C:LEU:H	1:52:C:ALA:H	1	0.2
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	7	0.2
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	13	0.2
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	14	0.2
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	15	0.2
(1,908)	1:43:C:ASP:H	1:63:C:THR:H	3	0.2
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	1	0.2
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	1	0.2
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	1	0.2
(1,885)	1:36:C:TRP:H	1:37:C:GLN:H	1	0.2
(1,866)	1:30:C:HIS:H	1:32:C:PHE:H	3	0.2
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	10	0.2
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	9	0.2
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	20	0.2
(1,707)	1:99:B:GLY:H	1:102:B:CYS:H	15	0.2
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	5	0.2
(1,697)	1:97:B:CYS:H	1:99:B:GLY:H	9	0.2
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	19	0.2
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	4	0.2
(1,623)	1:68:B:LEU:H	1:72:B:THR:H	8	0.2
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	11	0.2
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	20	0.2
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	3	0.2
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	11	0.2
(1,533)	1:50:B:GLN:H	1:51:B:LEU:H	12	0.2
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	17	0.2
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	17	0.2
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	17	0.2
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	17	0.2
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	17	0.2
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	17	0.2
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	17	0.2
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	17	0.2
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	2	0.2
(1,416)	1:14:B:GLN:H	1:84:B:PHE:HD1	15	0.2
(1,416)	1:14:B:GLN:H	1:84:B:PHE:HD2	15	0.2
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	15	0.2
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	12	0.2
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	19	0.2
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	9	0.2
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	13	0.2
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	2	0.2
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	3	0.2
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	9	0.2
(1,192)	1:62:A:VAL:HG11	1:63:A:THR:H	16	0.2
(1,192)	1:62:A:VAL:HG12	1:63:A:THR:H	16	0.2
(1,192)	1:62:A:VAL:HG13	1:63:A:THR:H	16	0.2
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	19	0.2
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	19	0.2
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	19	0.2
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD21	4	0.2
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD22	4	0.2
(1,90)	1:36:A:TRP:HZ3	1:68:A:LEU:HD23	4	0.2
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	2	0.2
(1,3)	1:10:A:THR:H	1:87:A:ALA:H	20	0.2
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG11	18	0.19
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG12	18	0.19
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG13	18	0.19
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG21	18	0.19
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG22	18	0.19
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG23	18	0.19
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG11	18	0.19
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG12	18	0.19
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG13	18	0.19
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG21	18	0.19
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG22	18	0.19
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG23	18	0.19
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG11	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG12	18	0.19
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG13	18	0.19
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG21	18	0.19
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG22	18	0.19
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG23	18	0.19
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	13	0.19
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	13	0.19
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	13	0.19
(1,1646)	1:89:C:ILE:HD11	2:451:G:VAL:HG11	13	0.19
(1,1646)	1:89:C:ILE:HD11	2:451:G:VAL:HG12	13	0.19
(1,1646)	1:89:C:ILE:HD11	2:451:G:VAL:HG13	13	0.19
(1,1646)	1:89:C:ILE:HD11	2:451:G:VAL:HG21	13	0.19
(1,1646)	1:89:C:ILE:HD11	2:451:G:VAL:HG22	13	0.19
(1,1646)	1:89:C:ILE:HD11	2:451:G:VAL:HG23	13	0.19
(1,1646)	1:89:C:ILE:HD12	2:451:G:VAL:HG11	13	0.19
(1,1646)	1:89:C:ILE:HD12	2:451:G:VAL:HG12	13	0.19
(1,1646)	1:89:C:ILE:HD12	2:451:G:VAL:HG13	13	0.19
(1,1646)	1:89:C:ILE:HD12	2:451:G:VAL:HG21	13	0.19
(1,1646)	1:89:C:ILE:HD12	2:451:G:VAL:HG22	13	0.19
(1,1646)	1:89:C:ILE:HD12	2:451:G:VAL:HG23	13	0.19
(1,1646)	1:89:C:ILE:HD13	2:451:G:VAL:HG11	13	0.19
(1,1646)	1:89:C:ILE:HD13	2:451:G:VAL:HG12	13	0.19
(1,1646)	1:89:C:ILE:HD13	2:451:G:VAL:HG13	13	0.19
(1,1646)	1:89:C:ILE:HD13	2:451:G:VAL:HG21	13	0.19
(1,1646)	1:89:C:ILE:HD13	2:451:G:VAL:HG22	13	0.19
(1,1646)	1:89:C:ILE:HD13	2:451:G:VAL:HG23	13	0.19
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG11	9	0.19
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG12	9	0.19
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG13	9	0.19
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG11	9	0.19
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG12	9	0.19
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG13	9	0.19
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG11	9	0.19
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG12	9	0.19
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG13	9	0.19
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD11	7	0.19
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD12	7	0.19
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD13	7	0.19
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD21	7	0.19
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD22	7	0.19
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD23	7	0.19
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD11	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD12	7	0.19
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD13	7	0.19
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD21	7	0.19
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD22	7	0.19
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD23	7	0.19
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD11	7	0.19
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD12	7	0.19
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD13	7	0.19
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD21	7	0.19
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD22	7	0.19
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD23	7	0.19
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD11	7	0.19
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD12	7	0.19
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD13	7	0.19
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD21	7	0.19
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD22	7	0.19
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD23	7	0.19
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD11	7	0.19
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD12	7	0.19
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD13	7	0.19
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD21	7	0.19
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD22	7	0.19
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD23	7	0.19
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD11	7	0.19
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD12	7	0.19
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD13	7	0.19
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD21	7	0.19
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD22	7	0.19
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD23	7	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	5	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	5	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	5	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	11	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	11	0.19
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	11	0.19
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	9	0.19
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	9	0.19
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	9	0.19
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	9	0.19
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	9	0.19
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	9	0.19
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE1	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE2	2	0.19
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE3	2	0.19
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE1	2	0.19
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE2	2	0.19
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE3	2	0.19
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE1	2	0.19
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE2	2	0.19
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE3	2	0.19
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	5	0.19
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	5	0.19
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	5	0.19
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	5	0.19
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	5	0.19
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	5	0.19
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG21	15	0.19
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG22	15	0.19
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG23	15	0.19
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG21	15	0.19
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG22	15	0.19
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG23	15	0.19
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG11	15	0.19
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG12	15	0.19
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG13	15	0.19
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG11	15	0.19
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG12	15	0.19
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG13	15	0.19
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG11	15	0.19
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG12	15	0.19
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG13	15	0.19
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	10	0.19
(1,1540)	1:126:D:LEU:H	1:127:D:ASN:H	2	0.19
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	4	0.19
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	4	0.19
(1,1463)	1:91:D:GLY:H	1:94:D:MET:H	7	0.19
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	4	0.19
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD21	4	0.19
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD22	4	0.19
(1,1425)	1:73:D:ALA:H	1:75:D:LEU:HD23	4	0.19
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	2	0.19
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	2	0.19
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	20	0.19
(1,1325)	1:49:D:SER:H	1:57:D:GLU:H	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	5	0.19
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD21	17	0.19
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD22	17	0.19
(1,1296)	1:42:D:LEU:HD21	1:128:D:LEU:HD23	17	0.19
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD21	17	0.19
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD22	17	0.19
(1,1296)	1:42:D:LEU:HD22	1:128:D:LEU:HD23	17	0.19
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD21	17	0.19
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD22	17	0.19
(1,1296)	1:42:D:LEU:HD23	1:128:D:LEU:HD23	17	0.19
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	7	0.19
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD21	10	0.19
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD22	10	0.19
(1,1287)	1:40:D:VAL:HG11	1:126:D:LEU:HD23	10	0.19
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD21	10	0.19
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD22	10	0.19
(1,1287)	1:40:D:VAL:HG12	1:126:D:LEU:HD23	10	0.19
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD21	10	0.19
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD22	10	0.19
(1,1287)	1:40:D:VAL:HG13	1:126:D:LEU:HD23	10	0.19
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	4	0.19
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	18	0.19
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	12	0.19
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	19	0.19
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	18	0.19
(1,1167)	1:128:C:LEU:HD21	1:129:C:ALA:H	20	0.19
(1,1167)	1:128:C:LEU:HD22	1:129:C:ALA:H	20	0.19
(1,1167)	1:128:C:LEU:HD23	1:129:C:ALA:H	20	0.19
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	9	0.19
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	9	0.19
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	9	0.19
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	8	0.19
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	18	0.19
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	4	0.19
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	5	0.19
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	6	0.19
(1,1107)	1:98:C:LEU:H	1:101:C:TYR:H	19	0.19
(1,1103)	1:97:C:CYS:H	1:100:C:ALA:H	3	0.19
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	16	0.19
(1,1073)	1:87:C:ALA:H	1:88:C:GLY:H	10	0.19
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	6	0.19
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:50:C:GLN:H	1:56:C:TYR:HE1	15	0.19
(1,939)	1:50:C:GLN:H	1:56:C:TYR:HE2	15	0.19
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	11	0.19
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	11	0.19
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	15	0.19
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG21	17	0.19
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG22	17	0.19
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG23	17	0.19
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG21	17	0.19
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG22	17	0.19
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG23	17	0.19
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG21	17	0.19
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG22	17	0.19
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG23	17	0.19
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG11	15	0.19
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG12	15	0.19
(1,912)	1:44:C:LEU:HD11	1:131:C:VAL:HG13	15	0.19
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG11	15	0.19
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG12	15	0.19
(1,912)	1:44:C:LEU:HD12	1:131:C:VAL:HG13	15	0.19
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG11	15	0.19
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG12	15	0.19
(1,912)	1:44:C:LEU:HD13	1:131:C:VAL:HG13	15	0.19
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	1	0.19
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	1	0.19
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	1	0.19
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	20	0.19
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	20	0.19
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	20	0.19
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	15	0.19
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	12	0.19
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	12	0.19
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	12	0.19
(1,767)	1:134:B:ASP:H	1:136:B:LEU:H	14	0.19
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	15	0.19
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	10	0.19
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	1	0.19
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	7	0.19
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	13	0.19
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	20	0.19
(1,684)	1:94:B:MET:H	1:96:B:HIS:H	9	0.19
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE1	13	0.19
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE2	13	0.19
(1,677)	1:91:B:GLY:H	1:94:B:MET:HE3	13	0.19
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	3	0.19
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	3	0.19
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD21	18	0.19
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD22	18	0.19
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD23	18	0.19
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	1	0.19
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	9	0.19
(1,532)	1:49:B:SER:H	1:59:B:VAL:H	6	0.19
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	18	0.19
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE1	8	0.19
(1,512)	1:44:B:LEU:HD11	1:133:B:PHE:HE2	8	0.19
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE1	8	0.19
(1,512)	1:44:B:LEU:HD12	1:133:B:PHE:HE2	8	0.19
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE1	8	0.19
(1,512)	1:44:B:LEU:HD13	1:133:B:PHE:HE2	8	0.19
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD21	13	0.19
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD22	13	0.19
(1,503)	1:42:B:LEU:HD21	1:44:B:LEU:HD23	13	0.19
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD21	13	0.19
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD22	13	0.19
(1,503)	1:42:B:LEU:HD22	1:44:B:LEU:HD23	13	0.19
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD21	13	0.19
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD22	13	0.19
(1,503)	1:42:B:LEU:HD23	1:44:B:LEU:HD23	13	0.19
(1,474)	1:36:B:TRP:HE1	1:37:B:GLN:H	17	0.19
(1,474)	1:36:B:TRP:HE1	1:37:B:GLN:H	19	0.19
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	1	0.19
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	1	0.19
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	1	0.19
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	1	0.19
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	1	0.19
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	1	0.19
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	1	0.19
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	1	0.19
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	1	0.19
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	17	0.19
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	3	0.19
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	5	0.19
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:140:A:TYR:H	1:141:A:LEU:H	12	0.19
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	8	0.19
(1,356)	1:121:A:GLY:H	1:123:A:PHE:H	8	0.19
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	5	0.19
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	4	0.19
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	3	0.19
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	19	0.19
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	5	0.19
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	2	0.19
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	2	0.19
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	2	0.19
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	10	0.19
(1,183)	1:60:A:LEU:H	1:82:A:GLY:H	9	0.19
(1,176)	1:59:A:VAL:HG11	1:80:A:GLN:H	13	0.19
(1,176)	1:59:A:VAL:HG12	1:80:A:GLN:H	13	0.19
(1,176)	1:59:A:VAL:HG13	1:80:A:GLN:H	13	0.19
(1,164)	1:56:A:TYR:H	1:86:A:ILE:H	5	0.19
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	5	0.19
(1,131)	1:47:A:ALA:H	1:61:A:ARG:H	7	0.19
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	9	0.19
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	16	0.19
(1,124)	1:44:A:LEU:HD21	1:133:A:PHE:HE1	4	0.19
(1,124)	1:44:A:LEU:HD21	1:133:A:PHE:HE2	4	0.19
(1,124)	1:44:A:LEU:HD22	1:133:A:PHE:HE1	4	0.19
(1,124)	1:44:A:LEU:HD22	1:133:A:PHE:HE2	4	0.19
(1,124)	1:44:A:LEU:HD23	1:133:A:PHE:HE1	4	0.19
(1,124)	1:44:A:LEU:HD23	1:133:A:PHE:HE2	4	0.19
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	13	0.19
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	9	0.19
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE1	16	0.18
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE2	16	0.18
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE3	16	0.18
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE1	16	0.18
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE2	16	0.18
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE3	16	0.18
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE1	16	0.18
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE2	16	0.18
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE3	16	0.18
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG21	12	0.18
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG22	12	0.18
(1,1672)	1:56:D:TYR:HE1	2:452:H:VAL:HG23	12	0.18
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG21	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG22	12	0.18
(1,1672)	1:56:D:TYR:HE2	2:452:H:VAL:HG23	12	0.18
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD11	19	0.18
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD12	19	0.18
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD13	19	0.18
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD21	19	0.18
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD22	19	0.18
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD23	19	0.18
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD11	19	0.18
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD12	19	0.18
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD13	19	0.18
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD21	19	0.18
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD22	19	0.18
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD23	19	0.18
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD11	19	0.18
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD12	19	0.18
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD13	19	0.18
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD21	19	0.18
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD22	19	0.18
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD23	19	0.18
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD11	19	0.18
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD12	19	0.18
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD13	19	0.18
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD21	19	0.18
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD22	19	0.18
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD23	19	0.18
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD11	19	0.18
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD12	19	0.18
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD13	19	0.18
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD21	19	0.18
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD22	19	0.18
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD23	19	0.18
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD11	19	0.18
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD12	19	0.18
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD13	19	0.18
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD21	19	0.18
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD22	19	0.18
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD23	19	0.18
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB1	8	0.18
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB2	8	0.18
(1,1658)	1:40:C:VAL:HG11	2:467:G:ALA:HB3	8	0.18
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB1	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB2	8	0.18
(1,1658)	1:40:C:VAL:HG12	2:467:G:ALA:HB3	8	0.18
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB1	8	0.18
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB2	8	0.18
(1,1658)	1:40:C:VAL:HG13	2:467:G:ALA:HB3	8	0.18
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB1	8	0.18
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB2	8	0.18
(1,1658)	1:40:C:VAL:HG21	2:467:G:ALA:HB3	8	0.18
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB1	8	0.18
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB2	8	0.18
(1,1658)	1:40:C:VAL:HG22	2:467:G:ALA:HB3	8	0.18
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB1	8	0.18
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB2	8	0.18
(1,1658)	1:40:C:VAL:HG23	2:467:G:ALA:HB3	8	0.18
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD1	12	0.18
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD2	12	0.18
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD1	12	0.18
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD2	12	0.18
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD1	12	0.18
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD2	12	0.18
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD11	7	0.18
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD12	7	0.18
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD13	7	0.18
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD11	10	0.18
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD12	10	0.18
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD13	10	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD11	6	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD12	6	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD13	6	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD21	6	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD22	6	0.18
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD23	6	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD11	6	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD12	6	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD13	6	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD21	6	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD22	6	0.18
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD23	6	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD11	6	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD12	6	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD13	6	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD21	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD22	6	0.18
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD23	6	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD11	6	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD12	6	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD13	6	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD21	6	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD22	6	0.18
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD23	6	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD11	6	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD12	6	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD13	6	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD21	6	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD22	6	0.18
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD23	6	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD11	6	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD12	6	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD13	6	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD21	6	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD22	6	0.18
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD23	6	0.18
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG21	7	0.18
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG22	7	0.18
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG23	7	0.18
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG21	7	0.18
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG22	7	0.18
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG23	7	0.18
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	15	0.18
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	15	0.18
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	15	0.18
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	15	0.18
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	15	0.18
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	15	0.18
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	20	0.18
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	20	0.18
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	20	0.18
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	20	0.18
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	20	0.18
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	20	0.18
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD11	2	0.18
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD12	2	0.18
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD13	2	0.18
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD11	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD12	2	0.18
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD13	2	0.18
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD11	2	0.18
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD12	2	0.18
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD13	2	0.18
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	16	0.18
(1,1543)	1:127:D:ASN:H	1:128:D:LEU:H	2	0.18
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	9	0.18
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	10	0.18
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD11	16	0.18
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD12	16	0.18
(1,1474)	1:94:D:MET:HE1	1:98:D:LEU:HD13	16	0.18
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD11	16	0.18
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD12	16	0.18
(1,1474)	1:94:D:MET:HE2	1:98:D:LEU:HD13	16	0.18
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD11	16	0.18
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD12	16	0.18
(1,1474)	1:94:D:MET:HE3	1:98:D:LEU:HD13	16	0.18
(1,1472)	1:94:D:MET:H	1:96:D:HIS:H	6	0.18
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	19	0.18
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	20	0.18
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	2	0.18
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	11	0.18
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	17	0.18
(1,1313)	1:46:D:THR:H	1:61:D:ARG:H	1	0.18
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	11	0.18
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	1	0.18
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	7	0.18
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	2	0.18
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	10	0.18
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	13	0.18
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	14	0.18
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	14	0.18
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	4	0.18
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	14	0.18
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	13	0.18
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	20	0.18
(1,1208)	1:12:D:GLN:H	1:85:D:SER:H	13	0.18
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	19	0.18
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	19	0.18
(1,1189)	1:137:C:PHE:H	1:140:C:TYR:H	5	0.18
(1,1178)	1:134:C:ASP:H	1:136:C:LEU:H	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1163)	1:126:C:LEU:HD21	1:127:C:ASN:H	1	0.18
(1,1163)	1:126:C:LEU:HD22	1:127:C:ASN:H	1	0.18
(1,1163)	1:126:C:LEU:HD23	1:127:C:ASN:H	1	0.18
(1,1103)	1:97:C:CYS:H	1:100:C:ALA:H	10	0.18
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	20	0.18
(1,1094)	1:95:C:ALA:H	1:98:C:LEU:H	5	0.18
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	11	0.18
(1,1030)	1:68:C:LEU:H	1:73:C:ALA:H	19	0.18
(1,985)	1:60:C:LEU:H	1:81:C:GLY:H	5	0.18
(1,961)	1:55:C:VAL:H	1:86:C:ILE:H	3	0.18
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	2	0.18
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	5	0.18
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	14	0.18
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	8	0.18
(1,934)	1:49:C:SER:H	1:57:C:GLU:H	9	0.18
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	12	0.18
(1,921)	1:45:C:ASP:H	1:63:C:THR:H	11	0.18
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	2	0.18
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	2	0.18
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	2	0.18
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	15	0.18
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	15	0.18
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	15	0.18
(1,882)	1:33:C:GLN:H	1:34:C:LYS:H	20	0.18
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	8	0.18
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	10	0.18
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	14	0.18
(1,757)	1:127:B:ASN:H	1:128:B:LEU:H	4	0.18
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	13	0.18
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	13	0.18
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	13	0.18
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	13	0.18
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	13	0.18
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	13	0.18
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	13	0.18
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	13	0.18
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	13	0.18
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD21	1	0.18
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD22	1	0.18
(1,747)	1:118:B:VAL:HG21	1:126:B:LEU:HD23	1	0.18
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD21	1	0.18
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD22	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:118:B:VAL:HG22	1:126:B:LEU:HD23	1	0.18
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD21	1	0.18
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD22	1	0.18
(1,747)	1:118:B:VAL:HG23	1:126:B:LEU:HD23	1	0.18
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	7	0.18
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	17	0.18
(1,708)	1:100:B:ALA:H	1:101:B:TYR:H	12	0.18
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	1	0.18
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	9	0.18
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	12	0.18
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	12	0.18
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	19	0.18
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	8	0.18
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	8	0.18
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD11	19	0.18
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD12	19	0.18
(1,643)	1:74:B:PHE:HE1	1:126:B:LEU:HD13	19	0.18
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD11	19	0.18
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD12	19	0.18
(1,643)	1:74:B:PHE:HE2	1:126:B:LEU:HD13	19	0.18
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD21	11	0.18
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD22	11	0.18
(1,635)	1:73:B:ALA:H	1:75:B:LEU:HD23	11	0.18
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	1	0.18
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	19	0.18
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	11	0.18
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	11	0.18
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	11	0.18
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	11	0.18
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	11	0.18
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	11	0.18
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	11	0.18
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	11	0.18
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	11	0.18
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	9	0.18
(1,533)	1:50:B:GLN:H	1:51:B:LEU:H	2	0.18
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	2	0.18
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	2	0.18
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	2	0.18
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	2	0.18
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	2	0.18
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	2	0.18
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	2	0.18
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	2	0.18
(1,474)	1:36:B:TRP:HE1	1:37:B:GLN:H	3	0.18
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	1	0.18
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	13	0.18
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	7	0.18
(1,359)	1:122:A:THR:H	1:18:B:THR:H	18	0.18
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	19	0.18
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	4	0.18
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	19	0.18
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	12	0.18
(1,266)	1:85:A:SER:H	1:86:A:ILE:H	5	0.18
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	4	0.18
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	6	0.18
(1,177)	1:59:A:VAL:HG11	1:81:A:GLY:H	12	0.18
(1,177)	1:59:A:VAL:HG12	1:81:A:GLY:H	12	0.18
(1,177)	1:59:A:VAL:HG13	1:81:A:GLY:H	12	0.18
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	17	0.18
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	5	0.18
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	10	0.18
(1,106)	1:42:A:LEU:HD11	1:62:A:VAL:HG11	4	0.18
(1,106)	1:42:A:LEU:HD11	1:62:A:VAL:HG12	4	0.18
(1,106)	1:42:A:LEU:HD11	1:62:A:VAL:HG13	4	0.18
(1,106)	1:42:A:LEU:HD12	1:62:A:VAL:HG11	4	0.18
(1,106)	1:42:A:LEU:HD12	1:62:A:VAL:HG12	4	0.18
(1,106)	1:42:A:LEU:HD12	1:62:A:VAL:HG13	4	0.18
(1,106)	1:42:A:LEU:HD13	1:62:A:VAL:HG11	4	0.18
(1,106)	1:42:A:LEU:HD13	1:62:A:VAL:HG12	4	0.18
(1,106)	1:42:A:LEU:HD13	1:62:A:VAL:HG13	4	0.18
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	5	0.18
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	8	0.18
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	11	0.18
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	10	0.18
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	12	0.18
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG11	2	0.17
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG12	2	0.17
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG13	2	0.17
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG11	2	0.17
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG12	2	0.17
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG13	2	0.17
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG11	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG12	2	0.17
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG13	2	0.17
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG11	9	0.17
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG12	9	0.17
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG13	9	0.17
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG21	9	0.17
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG22	9	0.17
(1,1674)	1:86:D:ILE:HD11	2:451:H:VAL:HG23	9	0.17
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG11	9	0.17
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG12	9	0.17
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG13	9	0.17
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG21	9	0.17
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG22	9	0.17
(1,1674)	1:86:D:ILE:HD12	2:451:H:VAL:HG23	9	0.17
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG11	9	0.17
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG12	9	0.17
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG13	9	0.17
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG21	9	0.17
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG22	9	0.17
(1,1674)	1:86:D:ILE:HD13	2:451:H:VAL:HG23	9	0.17
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	9	0.17
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	9	0.17
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	9	0.17
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE1	14	0.17
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE2	14	0.17
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE3	14	0.17
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE1	14	0.17
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE2	14	0.17
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE3	14	0.17
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE1	14	0.17
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE2	14	0.17
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE3	14	0.17
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB1	1	0.17
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB2	1	0.17
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB3	1	0.17
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB1	1	0.17
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB2	1	0.17
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB3	1	0.17
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB1	1	0.17
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB2	1	0.17
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB3	1	0.17
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB1	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB2	1	0.17
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB3	1	0.17
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB1	1	0.17
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB2	1	0.17
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB3	1	0.17
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB1	1	0.17
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB2	1	0.17
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB3	1	0.17
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG11	3	0.17
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG12	3	0.17
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG13	3	0.17
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG11	3	0.17
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG12	3	0.17
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG13	3	0.17
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG11	3	0.17
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG12	3	0.17
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG13	3	0.17
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	2	0.17
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	2	0.17
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	2	0.17
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	2	0.17
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	2	0.17
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	2	0.17
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	8	0.17
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	8	0.17
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	8	0.17
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	8	0.17
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	8	0.17
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	8	0.17
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB1	13	0.17
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB2	13	0.17
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB3	13	0.17
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB1	13	0.17
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB2	13	0.17
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB3	13	0.17
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB1	13	0.17
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB2	13	0.17
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB3	13	0.17
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB1	13	0.17
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB2	13	0.17
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB3	13	0.17
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB1	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB2	13	0.17
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB3	13	0.17
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB1	13	0.17
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB2	13	0.17
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB3	13	0.17
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG11	10	0.17
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG12	10	0.17
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG13	10	0.17
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG21	10	0.17
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG22	10	0.17
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG23	10	0.17
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG11	10	0.17
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG12	10	0.17
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG13	10	0.17
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG21	10	0.17
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG22	10	0.17
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG23	10	0.17
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG11	10	0.17
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG12	10	0.17
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG13	10	0.17
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG21	10	0.17
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG22	10	0.17
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG23	10	0.17
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD11	19	0.17
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD12	19	0.17
(1,1556)	1:133:D:PHE:HD1	1:136:D:LEU:HD13	19	0.17
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD11	19	0.17
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD12	19	0.17
(1,1556)	1:133:D:PHE:HD2	1:136:D:LEU:HD13	19	0.17
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	15	0.17
(1,1495)	1:100:D:ALA:H	1:102:D:CYS:H	7	0.17
(1,1490)	1:99:D:GLY:H	1:100:D:ALA:H	20	0.17
(1,1472)	1:94:D:MET:H	1:96:D:HIS:H	13	0.17
(1,1467)	1:92:D:THR:H	1:95:D:ALA:H	8	0.17
(1,1456)	1:87:D:ALA:H	1:89:D:ILE:H	10	0.17
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD21	3	0.17
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD22	3	0.17
(1,1433)	1:74:D:PHE:HE1	1:126:D:LEU:HD23	3	0.17
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD21	3	0.17
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD22	3	0.17
(1,1433)	1:74:D:PHE:HE2	1:126:D:LEU:HD23	3	0.17
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1414)	1:68:D:LEU:H	1:71:D:GLU:H	6	0.17
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD21	2	0.17
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD22	2	0.17
(1,1397)	1:64:D:VAL:HG21	1:126:D:LEU:HD23	2	0.17
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD21	2	0.17
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD22	2	0.17
(1,1397)	1:64:D:VAL:HG22	1:126:D:LEU:HD23	2	0.17
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD21	2	0.17
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD22	2	0.17
(1,1397)	1:64:D:VAL:HG23	1:126:D:LEU:HD23	2	0.17
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD21	13	0.17
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD22	13	0.17
(1,1395)	1:64:D:VAL:HG11	1:126:D:LEU:HD23	13	0.17
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD21	13	0.17
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD22	13	0.17
(1,1395)	1:64:D:VAL:HG12	1:126:D:LEU:HD23	13	0.17
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD21	13	0.17
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD22	13	0.17
(1,1395)	1:64:D:VAL:HG13	1:126:D:LEU:HD23	13	0.17
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	18	0.17
(1,1351)	1:56:D:TYR:HD1	1:57:D:GLU:H	12	0.17
(1,1351)	1:56:D:TYR:HD2	1:57:D:GLU:H	12	0.17
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	5	0.17
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	14	0.17
(1,1317)	1:47:D:ALA:H	1:61:D:ARG:H	19	0.17
(1,1309)	1:45:D:ASP:H	1:46:D:THR:H	3	0.17
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	8	0.17
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	17	0.17
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	17	0.17
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	14	0.17
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	11	0.17
(1,1216)	1:15:D:ARG:H	1:83:D:ILE:H	17	0.17
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	14	0.17
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	15	0.17
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	6	0.17
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	15	0.17
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	19	0.17
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	20	0.17
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	7	0.17
(1,1103)	1:97:C:CYS:H	1:100:C:ALA:H	13	0.17
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	13	0.17
(1,1090)	1:94:C:MET:H	1:96:C:HIS:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:87:C:ALA:H	1:88:C:GLY:H	8	0.17
(1,1055)	1:77:C:GLU:H	1:78:C:VAL:H	11	0.17
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	7	0.17
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	7	0.17
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	7	0.17
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	7	0.17
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	7	0.17
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	7	0.17
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	7	0.17
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	7	0.17
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	7	0.17
(1,977)	1:58:C:VAL:HG21	1:98:C:LEU:HD21	1	0.17
(1,977)	1:58:C:VAL:HG21	1:98:C:LEU:HD22	1	0.17
(1,977)	1:58:C:VAL:HG21	1:98:C:LEU:HD23	1	0.17
(1,977)	1:58:C:VAL:HG22	1:98:C:LEU:HD21	1	0.17
(1,977)	1:58:C:VAL:HG22	1:98:C:LEU:HD22	1	0.17
(1,977)	1:58:C:VAL:HG22	1:98:C:LEU:HD23	1	0.17
(1,977)	1:58:C:VAL:HG23	1:98:C:LEU:HD21	1	0.17
(1,977)	1:58:C:VAL:HG23	1:98:C:LEU:HD22	1	0.17
(1,977)	1:58:C:VAL:HG23	1:98:C:LEU:HD23	1	0.17
(1,945)	1:51:C:LEU:H	1:56:C:TYR:HD1	17	0.17
(1,945)	1:51:C:LEU:H	1:56:C:TYR:HD2	17	0.17
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	3	0.17
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	18	0.17
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD21	7	0.17
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD22	7	0.17
(1,917)	1:44:C:LEU:HD21	1:128:C:LEU:HD23	7	0.17
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD21	7	0.17
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD22	7	0.17
(1,917)	1:44:C:LEU:HD22	1:128:C:LEU:HD23	7	0.17
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD21	7	0.17
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD22	7	0.17
(1,917)	1:44:C:LEU:HD23	1:128:C:LEU:HD23	7	0.17
(1,910)	1:43:C:ASP:H	1:65:C:THR:H	7	0.17
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD11	19	0.17
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD12	19	0.17
(1,903)	1:42:C:LEU:HD11	1:128:C:LEU:HD13	19	0.17
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD11	19	0.17
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD12	19	0.17
(1,903)	1:42:C:LEU:HD12	1:128:C:LEU:HD13	19	0.17
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD11	19	0.17
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD12	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,903)	1:42:C:LEU:HD13	1:128:C:LEU:HD13	19	0.17
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	8	0.17
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	16	0.17
(1,895)	1:41:C:LYS:H	1:42:C:LEU:H	4	0.17
(1,866)	1:30:C:HIS:H	1:32:C:PHE:H	5	0.17
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	7	0.17
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	8	0.17
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	10	0.17
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	2	0.17
(1,792)	1:9:C:MET:HE1	1:97:C:CYS:H	19	0.17
(1,792)	1:9:C:MET:HE2	1:97:C:CYS:H	19	0.17
(1,792)	1:9:C:MET:HE3	1:97:C:CYS:H	19	0.17
(1,767)	1:134:B:ASP:H	1:136:B:LEU:H	13	0.17
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	4	0.17
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	2	0.17
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	12	0.17
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	20	0.17
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	10	0.17
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	16	0.17
(1,685)	1:94:B:MET:H	1:97:B:CYS:H	9	0.17
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	19	0.17
(1,668)	1:87:B:ALA:H	1:89:B:ILE:H	5	0.17
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	2	0.17
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	12	0.17
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD11	4	0.17
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD12	4	0.17
(1,556)	1:56:B:TYR:H	1:98:B:LEU:HD13	4	0.17
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD11	1	0.17
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD12	1	0.17
(1,484)	1:40:B:VAL:HG11	1:126:B:LEU:HD13	1	0.17
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD11	1	0.17
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD12	1	0.17
(1,484)	1:40:B:VAL:HG12	1:126:B:LEU:HD13	1	0.17
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD11	1	0.17
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD12	1	0.17
(1,484)	1:40:B:VAL:HG13	1:126:B:LEU:HD13	1	0.17
(1,474)	1:36:B:TRP:HE1	1:37:B:GLN:H	1	0.17
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	6	0.17
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	6	0.17
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	6	0.17
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	6	0.17
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	6	0.17
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	6	0.17
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	6	0.17
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	6	0.17
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	6	0.17
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	6	0.17
(1,395)	1:140:A:TYR:H	1:141:A:LEU:H	7	0.17
(1,395)	1:140:A:TYR:H	1:141:A:LEU:H	16	0.17
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	7	0.17
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	11	0.17
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	7	0.17
(1,305)	1:98:A:LEU:HD11	1:99:A:GLY:H	20	0.17
(1,305)	1:98:A:LEU:HD12	1:99:A:GLY:H	20	0.17
(1,305)	1:98:A:LEU:HD13	1:99:A:GLY:H	20	0.17
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	7	0.17
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	9	0.17
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	13	0.17
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	12	0.17
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	16	0.17
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	2	0.17
(1,302)	1:98:A:LEU:H	1:100:A:ALA:H	6	0.17
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	3	0.17
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	18	0.17
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	10	0.17
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	12	0.17
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	8	0.17
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	14	0.17
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	14	0.17
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	14	0.17
(1,223)	1:68:A:LEU:H	1:70:A:GLU:H	7	0.17
(1,222)	1:68:A:LEU:H	1:69:A:GLY:H	19	0.17
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	1	0.17
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG21	10	0.17
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG22	10	0.17
(1,112)	1:42:A:LEU:HD21	1:131:A:VAL:HG23	10	0.17
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG21	10	0.17
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG22	10	0.17
(1,112)	1:42:A:LEU:HD22	1:131:A:VAL:HG23	10	0.17
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG21	10	0.17
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG22	10	0.17
(1,112)	1:42:A:LEU:HD23	1:131:A:VAL:HG23	10	0.17
(1,111)	1:42:A:LEU:HD21	1:129:A:ALA:H	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:42:A:LEU:HD22	1:129:A:ALA:H	20	0.17
(1,111)	1:42:A:LEU:HD23	1:129:A:ALA:H	20	0.17
(1,101)	1:41:A:LYS:H	1:42:A:LEU:H	17	0.17
(1,97)	1:39:A:GLU:H	1:67:A:SER:H	11	0.17
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	2	0.17
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	10	0.17
(1,18)	1:14:A:GLN:H	1:83:A:ILE:H	15	0.17
(1,1689)	1:98:D:LEU:HD11	2:454:H:LEU:HD11	17	0.16
(1,1689)	1:98:D:LEU:HD11	2:454:H:LEU:HD12	17	0.16
(1,1689)	1:98:D:LEU:HD11	2:454:H:LEU:HD13	17	0.16
(1,1689)	1:98:D:LEU:HD11	2:454:H:LEU:HD21	17	0.16
(1,1689)	1:98:D:LEU:HD11	2:454:H:LEU:HD22	17	0.16
(1,1689)	1:98:D:LEU:HD11	2:454:H:LEU:HD23	17	0.16
(1,1689)	1:98:D:LEU:HD12	2:454:H:LEU:HD11	17	0.16
(1,1689)	1:98:D:LEU:HD12	2:454:H:LEU:HD12	17	0.16
(1,1689)	1:98:D:LEU:HD12	2:454:H:LEU:HD13	17	0.16
(1,1689)	1:98:D:LEU:HD12	2:454:H:LEU:HD21	17	0.16
(1,1689)	1:98:D:LEU:HD12	2:454:H:LEU:HD22	17	0.16
(1,1689)	1:98:D:LEU:HD12	2:454:H:LEU:HD23	17	0.16
(1,1689)	1:98:D:LEU:HD13	2:454:H:LEU:HD11	17	0.16
(1,1689)	1:98:D:LEU:HD13	2:454:H:LEU:HD12	17	0.16
(1,1689)	1:98:D:LEU:HD13	2:454:H:LEU:HD13	17	0.16
(1,1689)	1:98:D:LEU:HD13	2:454:H:LEU:HD21	17	0.16
(1,1689)	1:98:D:LEU:HD13	2:454:H:LEU:HD22	17	0.16
(1,1689)	1:98:D:LEU:HD13	2:454:H:LEU:HD23	17	0.16
(1,1689)	1:98:D:LEU:HD21	2:454:H:LEU:HD11	17	0.16
(1,1689)	1:98:D:LEU:HD21	2:454:H:LEU:HD12	17	0.16
(1,1689)	1:98:D:LEU:HD21	2:454:H:LEU:HD13	17	0.16
(1,1689)	1:98:D:LEU:HD21	2:454:H:LEU:HD21	17	0.16
(1,1689)	1:98:D:LEU:HD21	2:454:H:LEU:HD22	17	0.16
(1,1689)	1:98:D:LEU:HD21	2:454:H:LEU:HD23	17	0.16
(1,1689)	1:98:D:LEU:HD22	2:454:H:LEU:HD11	17	0.16
(1,1689)	1:98:D:LEU:HD22	2:454:H:LEU:HD12	17	0.16
(1,1689)	1:98:D:LEU:HD22	2:454:H:LEU:HD13	17	0.16
(1,1689)	1:98:D:LEU:HD22	2:454:H:LEU:HD21	17	0.16
(1,1689)	1:98:D:LEU:HD22	2:454:H:LEU:HD22	17	0.16
(1,1689)	1:98:D:LEU:HD22	2:454:H:LEU:HD23	17	0.16
(1,1689)	1:98:D:LEU:HD23	2:454:H:LEU:HD11	17	0.16
(1,1689)	1:98:D:LEU:HD23	2:454:H:LEU:HD12	17	0.16
(1,1689)	1:98:D:LEU:HD23	2:454:H:LEU:HD13	17	0.16
(1,1689)	1:98:D:LEU:HD23	2:454:H:LEU:HD21	17	0.16
(1,1689)	1:98:D:LEU:HD23	2:454:H:LEU:HD22	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1689)	1:98:D:LEU:HD23	2:454:H:LEU:HD23	17	0.16
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD11	14	0.16
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD12	14	0.16
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD13	14	0.16
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD21	14	0.16
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD22	14	0.16
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD23	14	0.16
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD11	14	0.16
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD12	14	0.16
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD13	14	0.16
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD21	14	0.16
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD22	14	0.16
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD23	14	0.16
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD11	14	0.16
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD12	14	0.16
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD13	14	0.16
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD21	14	0.16
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD22	14	0.16
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD23	14	0.16
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD11	14	0.16
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD12	14	0.16
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD13	14	0.16
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD21	14	0.16
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD22	14	0.16
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD23	14	0.16
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD11	14	0.16
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD12	14	0.16
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD13	14	0.16
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD21	14	0.16
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD22	14	0.16
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD23	14	0.16
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD11	14	0.16
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD12	14	0.16
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD13	14	0.16
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD21	14	0.16
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD22	14	0.16
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD23	14	0.16
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE1	9	0.16
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE2	9	0.16
(1,1684)	1:128:D:LEU:HD11	2:464:H:MET:HE3	9	0.16
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE1	9	0.16
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1684)	1:128:D:LEU:HD12	2:464:H:MET:HE3	9	0.16
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE1	9	0.16
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE2	9	0.16
(1,1684)	1:128:D:LEU:HD13	2:464:H:MET:HE3	9	0.16
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	17	0.16
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	17	0.16
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	17	0.16
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	17	0.16
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	17	0.16
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	17	0.16
(1,1677)	1:44:D:LEU:HD11	2:460:H:LEU:HD11	19	0.16
(1,1677)	1:44:D:LEU:HD11	2:460:H:LEU:HD12	19	0.16
(1,1677)	1:44:D:LEU:HD11	2:460:H:LEU:HD13	19	0.16
(1,1677)	1:44:D:LEU:HD12	2:460:H:LEU:HD11	19	0.16
(1,1677)	1:44:D:LEU:HD12	2:460:H:LEU:HD12	19	0.16
(1,1677)	1:44:D:LEU:HD12	2:460:H:LEU:HD13	19	0.16
(1,1677)	1:44:D:LEU:HD13	2:460:H:LEU:HD11	19	0.16
(1,1677)	1:44:D:LEU:HD13	2:460:H:LEU:HD12	19	0.16
(1,1677)	1:44:D:LEU:HD13	2:460:H:LEU:HD13	19	0.16
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	14	0.16
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	14	0.16
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	14	0.16
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	15	0.16
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	15	0.16
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	15	0.16
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	15	0.16
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	15	0.16
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	15	0.16
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	16	0.16
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	16	0.16
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	16	0.16
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	16	0.16
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	16	0.16
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	16	0.16
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD11	19	0.16
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD12	19	0.16
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD13	19	0.16
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD11	19	0.16
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD12	19	0.16
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD13	19	0.16
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD11	19	0.16
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD12	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD13	19	0.16
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB1	12	0.16
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB2	12	0.16
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB3	12	0.16
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB1	12	0.16
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB2	12	0.16
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB3	12	0.16
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB1	12	0.16
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB2	12	0.16
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB3	12	0.16
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB1	12	0.16
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB2	12	0.16
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB3	12	0.16
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB1	12	0.16
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB2	12	0.16
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB3	12	0.16
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB1	12	0.16
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB2	12	0.16
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB3	12	0.16
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD11	15	0.16
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD12	15	0.16
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD13	15	0.16
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD11	15	0.16
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD12	15	0.16
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD13	15	0.16
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD11	15	0.16
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD12	15	0.16
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD13	15	0.16
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	7	0.16
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	7	0.16
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	7	0.16
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	7	0.16
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	7	0.16
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	7	0.16
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD11	12	0.16
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD12	12	0.16
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD13	12	0.16
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	13	0.16
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	13	0.16
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	13	0.16
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	13	0.16
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	13	0.16
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	13	0.16
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	13	0.16
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	13	0.16
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	13	0.16
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	13	0.16
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	13	0.16
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	13	0.16
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	13	0.16
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	13	0.16
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	13	0.16
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	13	0.16
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	13	0.16
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	13	0.16
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	13	0.16
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	13	0.16
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	13	0.16
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	13	0.16
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	13	0.16
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	13	0.16
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	13	0.16
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	13	0.16
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	13	0.16
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	13	0.16
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	13	0.16
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	13	0.16
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	13	0.16
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	13	0.16
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	13	0.16
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	13	0.16
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	13	0.16
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	2	0.16
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	2	0.16
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	2	0.16
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	2	0.16
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	2	0.16
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	2	0.16
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG11	20	0.16
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG12	20	0.16
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG13	20	0.16
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG11	20	0.16
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG12	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG13	20	0.16
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG11	20	0.16
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG12	20	0.16
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG13	20	0.16
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD11	10	0.16
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD12	10	0.16
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD13	10	0.16
(1,1578)	1:139:D:ASN:H	1:141:D:LEU:H	8	0.16
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	17	0.16
(1,1488)	1:98:D:LEU:H	1:100:D:ALA:H	7	0.16
(1,1488)	1:98:D:LEU:H	1:100:D:ALA:H	12	0.16
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	11	0.16
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	15	0.16
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	13	0.16
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	13	0.16
(1,1325)	1:49:D:SER:H	1:57:D:GLU:H	9	0.16
(1,1298)	1:43:D:ASP:H	1:44:D:LEU:H	11	0.16
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	8	0.16
(1,1271)	1:35:D:ASP:H	1:36:D:TRP:H	6	0.16
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	6	0.16
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	16	0.16
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	1	0.16
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	1	0.16
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	1	0.16
(1,1230)	1:20:D:ASP:H	1:79:D:GLN:H	19	0.16
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	19	0.16
(1,1213)	1:14:D:GLN:H	1:84:D:PHE:HD1	2	0.16
(1,1213)	1:14:D:GLN:H	1:84:D:PHE:HD2	2	0.16
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	6	0.16
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	8	0.16
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	15	0.16
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	3	0.16
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	3	0.16
(1,1178)	1:134:C:ASP:H	1:136:C:LEU:H	11	0.16
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	7	0.16
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	1	0.16
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	5	0.16
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	11	0.16
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	13	0.16
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	17	0.16
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	17	0.16
(1,1090)	1:94:C:MET:H	1:96:C:HIS:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1074)	1:87:C:ALA:H	1:89:C:ILE:H	15	0.16
(1,1073)	1:87:C:ALA:H	1:88:C:GLY:H	5	0.16
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	4	0.16
(1,961)	1:55:C:VAL:H	1:86:C:ILE:H	18	0.16
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	20	0.16
(1,938)	1:50:C:GLN:H	1:56:C:TYR:HD1	15	0.16
(1,938)	1:50:C:GLN:H	1:56:C:TYR:HD2	15	0.16
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	9	0.16
(1,908)	1:43:C:ASP:H	1:63:C:THR:H	14	0.16
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	17	0.16
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	7	0.16
(1,844)	1:22:C:SER:H	1:23:D:PHE:H	3	0.16
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	18	0.16
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	19	0.16
(1,793)	1:10:C:THR:H	1:11:C:PHE:H	18	0.16
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	13	0.16
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	7	0.16
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	15	0.16
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	5	0.16
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	10	0.16
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	11	0.16
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	8	0.16
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	10	0.16
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	13	0.16
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	3	0.16
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	3	0.16
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	3	0.16
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	3	0.16
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	3	0.16
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	3	0.16
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	3	0.16
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	3	0.16
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	3	0.16
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	7	0.16
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD11	7	0.16
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD12	7	0.16
(1,558)	1:56:B:TYR:HD1	1:98:B:LEU:HD13	7	0.16
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD11	7	0.16
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD12	7	0.16
(1,558)	1:56:B:TYR:HD2	1:98:B:LEU:HD13	7	0.16
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD1	15	0.16
(1,550)	1:55:B:VAL:H	1:56:B:TYR:HD2	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	9	0.16
(1,535)	1:51:B:LEU:H	1:52:B:ALA:H	18	0.16
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	8	0.16
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	16	0.16
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	5	0.16
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	13	0.16
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	13	0.16
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG11	1	0.16
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG12	1	0.16
(1,511)	1:44:B:LEU:HD11	1:131:B:VAL:HG13	1	0.16
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG11	1	0.16
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG12	1	0.16
(1,511)	1:44:B:LEU:HD12	1:131:B:VAL:HG13	1	0.16
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG11	1	0.16
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG12	1	0.16
(1,511)	1:44:B:LEU:HD13	1:131:B:VAL:HG13	1	0.16
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	15	0.16
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	15	0.16
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	15	0.16
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	15	0.16
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	15	0.16
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	15	0.16
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	15	0.16
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	15	0.16
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	15	0.16
(1,410)	1:12:B:GLN:H	1:13:B:ILE:H	2	0.16
(1,398)	1:9:B:MET:HE1	1:10:B:THR:H	7	0.16
(1,398)	1:9:B:MET:HE2	1:10:B:THR:H	7	0.16
(1,398)	1:9:B:MET:HE3	1:10:B:THR:H	7	0.16
(1,344)	1:117:A:MET:HE1	1:21:B:ILE:H	1	0.16
(1,344)	1:117:A:MET:HE2	1:21:B:ILE:H	1	0.16
(1,344)	1:117:A:MET:HE3	1:21:B:ILE:H	1	0.16
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	1	0.16
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	2	0.16
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	10	0.16
(1,308)	1:99:A:GLY:H	1:101:A:TYR:H	6	0.16
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	20	0.16
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	10	0.16
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	14	0.16
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	17	0.16
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	18	0.16
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	7	0.16
(1,298)	1:97:A:CYS:H	1:99:A:GLY:H	7	0.16
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	2	0.16
(1,266)	1:85:A:SER:H	1:86:A:ILE:H	17	0.16
(1,236)	1:73:A:ALA:H	1:74:A:PHE:H	16	0.16
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	10	0.16
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	10	0.16
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	10	0.16
(1,209)	1:66:A:ALA:H	1:73:A:ALA:H	14	0.16
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	4	0.16
(1,177)	1:59:A:VAL:HG11	1:81:A:GLY:H	19	0.16
(1,177)	1:59:A:VAL:HG12	1:81:A:GLY:H	19	0.16
(1,177)	1:59:A:VAL:HG13	1:81:A:GLY:H	19	0.16
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	4	0.16
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	2	0.16
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	7	0.16
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG11	13	0.16
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG12	13	0.16
(1,114)	1:43:A:ASP:H	1:62:A:VAL:HG13	13	0.16
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG11	1	0.16
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG12	1	0.16
(1,102)	1:41:A:LYS:H	1:64:A:VAL:HG13	1	0.16
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD21	11	0.16
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD22	11	0.16
(1,88)	1:36:A:TRP:HE3	1:68:A:LEU:HD23	11	0.16
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	4	0.16
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	17	0.16
(1,26)	1:17:A:TYR:H	1:81:A:GLY:H	14	0.16
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	3	0.16
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	16	0.16
(1,1681)	1:131:D:VAL:HG11	2:462:H:TYR:HD1	14	0.15
(1,1681)	1:131:D:VAL:HG11	2:462:H:TYR:HD2	14	0.15
(1,1681)	1:131:D:VAL:HG12	2:462:H:TYR:HD1	14	0.15
(1,1681)	1:131:D:VAL:HG12	2:462:H:TYR:HD2	14	0.15
(1,1681)	1:131:D:VAL:HG13	2:462:H:TYR:HD1	14	0.15
(1,1681)	1:131:D:VAL:HG13	2:462:H:TYR:HD2	14	0.15
(1,1678)	1:133:D:PHE:HD1	2:460:H:LEU:HD11	1	0.15
(1,1678)	1:133:D:PHE:HD1	2:460:H:LEU:HD12	1	0.15
(1,1678)	1:133:D:PHE:HD1	2:460:H:LEU:HD13	1	0.15
(1,1678)	1:133:D:PHE:HD2	2:460:H:LEU:HD11	1	0.15
(1,1678)	1:133:D:PHE:HD2	2:460:H:LEU:HD12	1	0.15
(1,1678)	1:133:D:PHE:HD2	2:460:H:LEU:HD13	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG11	19	0.15
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG12	19	0.15
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG13	19	0.15
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG11	19	0.15
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG12	19	0.15
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG13	19	0.15
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG11	19	0.15
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG12	19	0.15
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG13	19	0.15
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	14	0.15
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	14	0.15
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	14	0.15
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	14	0.15
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	14	0.15
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	14	0.15
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD11	13	0.15
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD12	13	0.15
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD13	13	0.15
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE1	18	0.15
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE2	18	0.15
(1,1657)	1:128:C:LEU:HD11	2:464:G:MET:HE3	18	0.15
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE1	18	0.15
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE2	18	0.15
(1,1657)	1:128:C:LEU:HD12	2:464:G:MET:HE3	18	0.15
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE1	18	0.15
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE2	18	0.15
(1,1657)	1:128:C:LEU:HD13	2:464:G:MET:HE3	18	0.15
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD11	5	0.15
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD12	5	0.15
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD13	5	0.15
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD11	5	0.15
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD12	5	0.15
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD13	5	0.15
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD11	5	0.15
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD12	5	0.15
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD13	5	0.15
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD11	9	0.15
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD12	9	0.15
(1,1623)	1:44:B:LEU:HD11	2:460:F:LEU:HD13	9	0.15
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD11	9	0.15
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD12	9	0.15
(1,1623)	1:44:B:LEU:HD12	2:460:F:LEU:HD13	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD11	9	0.15
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD12	9	0.15
(1,1623)	1:44:B:LEU:HD13	2:460:F:LEU:HD13	9	0.15
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG11	11	0.15
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG12	11	0.15
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG13	11	0.15
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG11	11	0.15
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG12	11	0.15
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG13	11	0.15
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG11	11	0.15
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG12	11	0.15
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG13	11	0.15
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG11	14	0.15
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG12	14	0.15
(1,1617)	1:86:B:ILE:HD11	2:452:F:VAL:HG13	14	0.15
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG11	14	0.15
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG12	14	0.15
(1,1617)	1:86:B:ILE:HD12	2:452:F:VAL:HG13	14	0.15
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG11	14	0.15
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG12	14	0.15
(1,1617)	1:86:B:ILE:HD13	2:452:F:VAL:HG13	14	0.15
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	9	0.15
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	9	0.15
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	9	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	7	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	7	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	7	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	11	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	11	0.15
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	11	0.15
(1,1607)	1:126:A:LEU:HD11	2:468:E:LEU:HD11	2	0.15
(1,1607)	1:126:A:LEU:HD11	2:468:E:LEU:HD12	2	0.15
(1,1607)	1:126:A:LEU:HD11	2:468:E:LEU:HD13	2	0.15
(1,1607)	1:126:A:LEU:HD11	2:468:E:LEU:HD21	2	0.15
(1,1607)	1:126:A:LEU:HD11	2:468:E:LEU:HD22	2	0.15
(1,1607)	1:126:A:LEU:HD11	2:468:E:LEU:HD23	2	0.15
(1,1607)	1:126:A:LEU:HD12	2:468:E:LEU:HD11	2	0.15
(1,1607)	1:126:A:LEU:HD12	2:468:E:LEU:HD12	2	0.15
(1,1607)	1:126:A:LEU:HD12	2:468:E:LEU:HD13	2	0.15
(1,1607)	1:126:A:LEU:HD12	2:468:E:LEU:HD21	2	0.15
(1,1607)	1:126:A:LEU:HD12	2:468:E:LEU:HD22	2	0.15
(1,1607)	1:126:A:LEU:HD12	2:468:E:LEU:HD23	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:126:A:LEU:HD13	2:468:E:LEU:HD11	2	0.15
(1,1607)	1:126:A:LEU:HD13	2:468:E:LEU:HD12	2	0.15
(1,1607)	1:126:A:LEU:HD13	2:468:E:LEU:HD13	2	0.15
(1,1607)	1:126:A:LEU:HD13	2:468:E:LEU:HD21	2	0.15
(1,1607)	1:126:A:LEU:HD13	2:468:E:LEU:HD22	2	0.15
(1,1607)	1:126:A:LEU:HD13	2:468:E:LEU:HD23	2	0.15
(1,1607)	1:126:A:LEU:HD21	2:468:E:LEU:HD11	2	0.15
(1,1607)	1:126:A:LEU:HD21	2:468:E:LEU:HD12	2	0.15
(1,1607)	1:126:A:LEU:HD21	2:468:E:LEU:HD13	2	0.15
(1,1607)	1:126:A:LEU:HD21	2:468:E:LEU:HD21	2	0.15
(1,1607)	1:126:A:LEU:HD21	2:468:E:LEU:HD22	2	0.15
(1,1607)	1:126:A:LEU:HD21	2:468:E:LEU:HD23	2	0.15
(1,1607)	1:126:A:LEU:HD22	2:468:E:LEU:HD11	2	0.15
(1,1607)	1:126:A:LEU:HD22	2:468:E:LEU:HD12	2	0.15
(1,1607)	1:126:A:LEU:HD22	2:468:E:LEU:HD13	2	0.15
(1,1607)	1:126:A:LEU:HD22	2:468:E:LEU:HD21	2	0.15
(1,1607)	1:126:A:LEU:HD22	2:468:E:LEU:HD22	2	0.15
(1,1607)	1:126:A:LEU:HD22	2:468:E:LEU:HD23	2	0.15
(1,1607)	1:126:A:LEU:HD23	2:468:E:LEU:HD11	2	0.15
(1,1607)	1:126:A:LEU:HD23	2:468:E:LEU:HD12	2	0.15
(1,1607)	1:126:A:LEU:HD23	2:468:E:LEU:HD13	2	0.15
(1,1607)	1:126:A:LEU:HD23	2:468:E:LEU:HD21	2	0.15
(1,1607)	1:126:A:LEU:HD23	2:468:E:LEU:HD22	2	0.15
(1,1607)	1:126:A:LEU:HD23	2:468:E:LEU:HD23	2	0.15
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE1	14	0.15
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE2	14	0.15
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE3	14	0.15
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE1	14	0.15
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE2	14	0.15
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE3	14	0.15
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE1	14	0.15
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE2	14	0.15
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE3	14	0.15
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	9	0.15
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	3	0.15
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	3	0.15
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	19	0.15
(1,1506)	1:110:D:ALA:H	1:112:D:GLU:H	6	0.15
(1,1493)	1:99:D:GLY:H	1:102:D:CYS:H	10	0.15
(1,1471)	1:94:D:MET:H	1:95:D:ALA:H	15	0.15
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	4	0.15
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	20	0.15
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	1	0.15
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	6	0.15
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	3	0.15
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	7	0.15
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	10	0.15
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	10	0.15
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	5	0.15
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	20	0.15
(1,1208)	1:12:D:GLN:H	1:85:D:SER:H	11	0.15
(1,1206)	1:11:D:PHE:HE1	1:102:D:CYS:H	8	0.15
(1,1206)	1:11:D:PHE:HE2	1:102:D:CYS:H	8	0.15
(1,1195)	1:139:C:ASN:H	1:140:C:TYR:H	6	0.15
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	19	0.15
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	9	0.15
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	15	0.15
(1,1098)	1:96:C:HIS:H	1:98:C:LEU:H	3	0.15
(1,1094)	1:95:C:ALA:H	1:98:C:LEU:H	20	0.15
(1,1090)	1:94:C:MET:H	1:96:C:HIS:H	17	0.15
(1,1073)	1:87:C:ALA:H	1:88:C:GLY:H	15	0.15
(1,1055)	1:77:C:GLU:H	1:78:C:VAL:H	6	0.15
(1,1030)	1:68:C:LEU:H	1:73:C:ALA:H	6	0.15
(1,1016)	1:66:C:ALA:H	1:76:C:CYS:H	15	0.15
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	6	0.15
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	6	0.15
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	6	0.15
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	6	0.15
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	6	0.15
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	6	0.15
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	6	0.15
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	6	0.15
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	6	0.15
(1,961)	1:55:C:VAL:H	1:86:C:ILE:H	1	0.15
(1,951)	1:52:C:ALA:H	1:55:C:VAL:H	8	0.15
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	2	0.15
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	19	0.15
(1,927)	1:47:C:ALA:H	1:60:C:LEU:H	6	0.15
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	9	0.15
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	9	0.15
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	9	0.15
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	3	0.15
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	5	0.15
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	15	0.15
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	15	0.15
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	17	0.15
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	18	0.15
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	3	0.15
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	15	0.15
(1,764)	1:133:B:PHE:H	1:136:B:LEU:H	7	0.15
(1,762)	1:133:B:PHE:H	1:134:B:ASP:H	6	0.15
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	1	0.15
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	6	0.15
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	14	0.15
(1,708)	1:100:B:ALA:H	1:101:B:TYR:H	4	0.15
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	5	0.15
(1,684)	1:94:B:MET:H	1:96:B:HIS:H	13	0.15
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	17	0.15
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	17	0.15
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	17	0.15
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	8	0.15
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	15	0.15
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	5	0.15
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD21	5	0.15
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD22	5	0.15
(1,601)	1:64:B:VAL:HG11	1:128:B:LEU:HD23	5	0.15
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD21	5	0.15
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD22	5	0.15
(1,601)	1:64:B:VAL:HG12	1:128:B:LEU:HD23	5	0.15
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD21	5	0.15
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD22	5	0.15
(1,601)	1:64:B:VAL:HG13	1:128:B:LEU:HD23	5	0.15
(1,595)	1:64:B:VAL:H	1:76:B:CYS:H	2	0.15
(1,595)	1:64:B:VAL:H	1:76:B:CYS:H	12	0.15
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	15	0.15
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	4	0.15
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	4	0.15
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	4	0.15
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	4	0.15
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	4	0.15
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	4	0.15
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	4	0.15
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	4	0.15
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG11	4	0.15
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG12	4	0.15
(1,493)	1:41:B:LYS:H	1:64:B:VAL:HG13	4	0.15
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	7	0.15
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	7	0.15
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	7	0.15
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	7	0.15
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	7	0.15
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	7	0.15
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	7	0.15
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	7	0.15
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	7	0.15
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	1	0.15
(1,403)	1:10:B:THR:H	1:89:B:ILE:H	19	0.15
(1,383)	1:136:A:LEU:H	1:139:A:ASN:H	19	0.15
(1,354)	1:119:A:SER:H	1:123:A:PHE:H	13	0.15
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	3	0.15
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	11	0.15
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	20	0.15
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	6	0.15
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	1	0.15
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	3	0.15
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	2	0.15
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	2	0.15
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	4	0.15
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	16	0.15
(1,289)	1:95:A:ALA:H	1:98:A:LEU:H	2	0.15
(1,271)	1:88:A:GLY:H	1:89:A:ILE:H	19	0.15
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	8	0.15
(1,233)	1:70:A:GLU:H	1:71:A:GLU:H	14	0.15
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	18	0.15
(1,222)	1:68:A:LEU:H	1:69:A:GLY:H	11	0.15
(1,221)	1:67:A:SER:H	1:73:A:ALA:H	18	0.15
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	18	0.15
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	20	0.15
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	3	0.15
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	14	0.15
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	16	0.15
(1,174)	1:59:A:VAL:H	1:82:A:GLY:H	18	0.15
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	5	0.15
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	16	0.15
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	16	0.15
(1,103)	1:41:A:LYS:H	1:65:A:THR:H	11	0.15
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	3	0.15
(1,87)	1:36:A:TRP:HE3	1:37:A:GLN:H	9	0.15
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	9	0.15
(1,66)	1:28:A:ALA:H	1:30:A:HIS:H	8	0.15
(1,66)	1:28:A:ALA:H	1:30:A:HIS:H	15	0.15
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	5	0.15
(1,18)	1:14:A:GLN:H	1:83:A:ILE:H	1	0.15
(1,1680)	1:100:D:ALA:HB1	2:461:H:PHE:HZ	11	0.14
(1,1680)	1:100:D:ALA:HB2	2:461:H:PHE:HZ	11	0.14
(1,1680)	1:100:D:ALA:HB3	2:461:H:PHE:HZ	11	0.14
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	10	0.14
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	10	0.14
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	10	0.14
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD11	9	0.14
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD12	9	0.14
(1,1665)	1:74:D:PHE:HE1	2:470:H:LEU:HD13	9	0.14
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD11	9	0.14
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD12	9	0.14
(1,1665)	1:74:D:PHE:HE2	2:470:H:LEU:HD13	9	0.14
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD1	18	0.14
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD2	18	0.14
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD1	18	0.14
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD2	18	0.14
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD1	18	0.14
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD2	18	0.14
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG11	5	0.14
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG12	5	0.14
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG13	5	0.14
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG11	5	0.14
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG12	5	0.14
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG13	5	0.14
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG11	5	0.14
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG12	5	0.14
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG13	5	0.14
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG21	12	0.14
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG22	12	0.14
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG23	12	0.14
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG21	12	0.14
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG22	12	0.14
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG23	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD11	14	0.14
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD12	14	0.14
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD13	14	0.14
(1,1627)	1:131:B:VAL:HG11	2:462:F:TYR:HD1	20	0.14
(1,1627)	1:131:B:VAL:HG11	2:462:F:TYR:HD2	20	0.14
(1,1627)	1:131:B:VAL:HG12	2:462:F:TYR:HD1	20	0.14
(1,1627)	1:131:B:VAL:HG12	2:462:F:TYR:HD2	20	0.14
(1,1627)	1:131:B:VAL:HG13	2:462:F:TYR:HD1	20	0.14
(1,1627)	1:131:B:VAL:HG13	2:462:F:TYR:HD2	20	0.14
(1,1626)	1:100:B:ALA:HB1	2:461:F:PHE:HZ	10	0.14
(1,1626)	1:100:B:ALA:HB2	2:461:F:PHE:HZ	10	0.14
(1,1626)	1:100:B:ALA:HB3	2:461:F:PHE:HZ	10	0.14
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD11	15	0.14
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD12	15	0.14
(1,1613)	1:36:B:TRP:HE1	2:470:F:LEU:HD13	15	0.14
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	10	0.14
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	10	0.14
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	10	0.14
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	10	0.14
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	10	0.14
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	10	0.14
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE1	19	0.14
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE2	19	0.14
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE1	19	0.14
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE2	19	0.14
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE1	19	0.14
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE2	19	0.14
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD11	9	0.14
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD12	9	0.14
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD13	9	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD11	2	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD12	2	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD13	2	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD21	2	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD22	2	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD23	2	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD11	2	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD12	2	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD13	2	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD21	2	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD22	2	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD23	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD11	2	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD12	2	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD13	2	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD21	2	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD22	2	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD23	2	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD11	2	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD12	2	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD13	2	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD21	2	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD22	2	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD23	2	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD11	2	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD12	2	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD13	2	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD21	2	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD22	2	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD23	2	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD11	2	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD12	2	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD13	2	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD21	2	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD22	2	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD23	2	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD11	7	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD12	7	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD13	7	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD21	7	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD22	7	0.14
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD23	7	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD11	7	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD12	7	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD13	7	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD21	7	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD22	7	0.14
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD23	7	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD11	7	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD12	7	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD13	7	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD21	7	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD22	7	0.14
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD23	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD11	7	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD12	7	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD13	7	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD21	7	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD22	7	0.14
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD23	7	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD11	7	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD12	7	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD13	7	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD21	7	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD22	7	0.14
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD23	7	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD11	7	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD12	7	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD13	7	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD21	7	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD22	7	0.14
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD23	7	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	2	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	2	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	2	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	2	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	2	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	2	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	2	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	2	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	2	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	2	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	2	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	2	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	2	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	2	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	2	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	2	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	2	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	2	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	2	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	2	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	2	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	2	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	2	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	2	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	2	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	2	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	2	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	2	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	2	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	2	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	2	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	2	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	2	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	2	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	2	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	4	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	4	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	4	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	4	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	4	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	4	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	4	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	4	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	4	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	4	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	4	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	4	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	4	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	4	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	4	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	4	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	4	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	4	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	4	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	4	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	4	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	4	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	4	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	4	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	4	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	4	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	4	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	4	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	4	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	4	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	4	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	4	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	4	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	4	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	4	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	11	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	11	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	11	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	11	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	11	0.14
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	11	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	11	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	11	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	11	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	11	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	11	0.14
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	11	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	11	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	11	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	11	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	11	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	11	0.14
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	11	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	11	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	11	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	11	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	11	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	11	0.14
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	11	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	11	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	11	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	11	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	11	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	11	0.14
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	11	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	11	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	11	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	11	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	11	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	11	0.14
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD1	18	0.14
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD2	18	0.14
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD1	18	0.14
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD2	18	0.14
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD1	18	0.14
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD2	18	0.14
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	7	0.14
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	7	0.14
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	7	0.14
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	7	0.14
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	7	0.14
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	7	0.14
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG11	5	0.14
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG12	5	0.14
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG13	5	0.14
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG11	5	0.14
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG12	5	0.14
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG13	5	0.14
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG11	5	0.14
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG12	5	0.14
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG13	5	0.14
(1,1540)	1:126:D:LEU:H	1:127:D:ASN:H	17	0.14
(1,1506)	1:110:D:ALA:H	1:112:D:GLU:H	4	0.14
(1,1485)	1:97:D:CYS:H	1:100:D:ALA:H	13	0.14
(1,1477)	1:95:D:ALA:H	1:98:D:LEU:H	19	0.14
(1,1409)	1:67:D:SER:H	1:68:D:LEU:H	10	0.14
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	18	0.14
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE1	20	0.14
(1,1324)	1:49:D:SER:H	1:56:D:TYR:HE2	20	0.14
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	3	0.14
(1,1322)	1:49:D:SER:H	1:50:D:GLN:H	16	0.14
(1,1313)	1:46:D:THR:H	1:61:D:ARG:H	14	0.14
(1,1304)	1:44:D:LEU:HD11	1:45:D:ASP:H	20	0.14
(1,1304)	1:44:D:LEU:HD12	1:45:D:ASP:H	20	0.14
(1,1304)	1:44:D:LEU:HD13	1:45:D:ASP:H	20	0.14
(1,1291)	1:41:D:LYS:H	1:65:D:THR:H	1	0.14
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	13	0.14
(1,1253)	1:30:D:HIS:H	1:32:D:PHE:H	19	0.14
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	12	0.14
(1,1238)	1:23:D:PHE:HE1	1:24:D:GLU:H	12	0.14
(1,1238)	1:23:D:PHE:HE2	1:24:D:GLU:H	12	0.14
(1,1201)	1:10:D:THR:H	1:87:D:ALA:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:10:D:THR:H	1:87:D:ALA:H	17	0.14
(1,1189)	1:137:C:PHE:H	1:140:C:TYR:H	13	0.14
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	4	0.14
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	10	0.14
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	12	0.14
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	15	0.14
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	19	0.14
(1,1109)	1:99:C:GLY:H	1:100:C:ALA:H	16	0.14
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	7	0.14
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	15	0.14
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	3	0.14
(1,1006)	1:64:C:VAL:H	1:77:C:GLU:H	3	0.14
(1,973)	1:58:C:VAL:H	1:82:C:GLY:H	6	0.14
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	5	0.14
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	11	0.14
(1,942)	1:51:C:LEU:H	1:55:C:VAL:H	18	0.14
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	10	0.14
(1,934)	1:49:C:SER:H	1:57:C:GLU:H	7	0.14
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	16	0.14
(1,928)	1:47:C:ALA:H	1:61:C:ARG:H	17	0.14
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG21	12	0.14
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG22	12	0.14
(1,913)	1:44:C:LEU:HD11	1:131:C:VAL:HG23	12	0.14
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG21	12	0.14
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG22	12	0.14
(1,913)	1:44:C:LEU:HD12	1:131:C:VAL:HG23	12	0.14
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG21	12	0.14
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG22	12	0.14
(1,913)	1:44:C:LEU:HD13	1:131:C:VAL:HG23	12	0.14
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	15	0.14
(1,895)	1:41:C:LYS:H	1:42:C:LEU:H	3	0.14
(1,895)	1:41:C:LYS:H	1:42:C:LEU:H	16	0.14
(1,843)	1:22:C:SER:H	1:79:C:GLN:H	5	0.14
(1,841)	1:22:C:SER:H	1:78:C:VAL:H	2	0.14
(1,831)	1:19:C:LYS:H	1:81:C:GLY:H	3	0.14
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	14	0.14
(1,795)	1:10:C:THR:H	1:89:C:ILE:H	10	0.14
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	14	0.14
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	14	0.14
(1,697)	1:97:B:CYS:H	1:99:B:GLY:H	5	0.14
(1,697)	1:97:B:CYS:H	1:99:B:GLY:H	10	0.14
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	17	0.14
(1,679)	1:92:B:THR:H	1:94:B:MET:H	5	0.14
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	2	0.14
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	11	0.14
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	11	0.14
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	11	0.14
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	6	0.14
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	1	0.14
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	4	0.14
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	5	0.14
(1,533)	1:50:B:GLN:H	1:51:B:LEU:H	15	0.14
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	8	0.14
(1,522)	1:47:B:ALA:H	1:48:B:SER:H	10	0.14
(1,513)	1:44:B:LEU:HD21	1:45:B:ASP:H	20	0.14
(1,513)	1:44:B:LEU:HD22	1:45:B:ASP:H	20	0.14
(1,513)	1:44:B:LEU:HD23	1:45:B:ASP:H	20	0.14
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	15	0.14
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	15	0.14
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	15	0.14
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	15	0.14
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	15	0.14
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	15	0.14
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	15	0.14
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	15	0.14
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	15	0.14
(1,439)	1:23:B:PHE:H	1:24:B:GLU:H	4	0.14
(1,438)	1:22:B:SER:H	1:79:B:GLN:H	1	0.14
(1,419)	1:15:B:ARG:H	1:83:B:ILE:H	16	0.14
(1,415)	1:14:B:GLN:H	1:83:B:ILE:H	10	0.14
(1,410)	1:12:B:GLN:H	1:13:B:ILE:H	18	0.14
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	19	0.14
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	19	0.14
(1,395)	1:140:A:TYR:H	1:141:A:LEU:H	8	0.14
(1,359)	1:122:A:THR:H	1:18:B:THR:H	8	0.14
(1,335)	1:114:A:ILE:H	1:117:A:MET:H	13	0.14
(1,329)	1:112:A:GLU:H	1:109:C:TYR:HE1	16	0.14
(1,329)	1:112:A:GLU:H	1:109:C:TYR:HE2	16	0.14
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	14	0.14
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	15	0.14
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	17	0.14
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	18	0.14
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	3	0.14
(1,293)	1:96:A:HIS:H	1:97:A:CYS:H	20	0.14
(1,281)	1:93:A:GLN:H	1:95:A:ALA:H	13	0.14
(1,274)	1:90:A:GLU:H	1:94:A:MET:H	17	0.14
(1,228)	1:68:A:LEU:HD11	1:71:A:GLU:H	5	0.14
(1,228)	1:68:A:LEU:HD12	1:71:A:GLU:H	5	0.14
(1,228)	1:68:A:LEU:HD13	1:71:A:GLU:H	5	0.14
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	7	0.14
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	12	0.14
(1,192)	1:62:A:VAL:HG11	1:63:A:THR:H	17	0.14
(1,192)	1:62:A:VAL:HG12	1:63:A:THR:H	17	0.14
(1,192)	1:62:A:VAL:HG13	1:63:A:THR:H	17	0.14
(1,180)	1:59:A:VAL:HG21	1:82:A:GLY:H	5	0.14
(1,180)	1:59:A:VAL:HG22	1:82:A:GLY:H	5	0.14
(1,180)	1:59:A:VAL:HG23	1:82:A:GLY:H	5	0.14
(1,169)	1:58:A:VAL:H	1:84:A:PHE:H	4	0.14
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	4	0.14
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	19	0.14
(1,103)	1:41:A:LYS:H	1:65:A:THR:H	16	0.14
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	10	0.14
(1,69)	1:28:A:ALA:HB1	1:17:B:TYR:HE1	1	0.14
(1,69)	1:28:A:ALA:HB1	1:17:B:TYR:HE2	1	0.14
(1,69)	1:28:A:ALA:HB2	1:17:B:TYR:HE1	1	0.14
(1,69)	1:28:A:ALA:HB2	1:17:B:TYR:HE2	1	0.14
(1,69)	1:28:A:ALA:HB3	1:17:B:TYR:HE1	1	0.14
(1,69)	1:28:A:ALA:HB3	1:17:B:TYR:HE2	1	0.14
(1,69)	1:28:A:ALA:HB1	1:17:B:TYR:HE1	16	0.14
(1,69)	1:28:A:ALA:HB1	1:17:B:TYR:HE2	16	0.14
(1,69)	1:28:A:ALA:HB2	1:17:B:TYR:HE1	16	0.14
(1,69)	1:28:A:ALA:HB2	1:17:B:TYR:HE2	16	0.14
(1,69)	1:28:A:ALA:HB3	1:17:B:TYR:HE1	16	0.14
(1,69)	1:28:A:ALA:HB3	1:17:B:TYR:HE2	16	0.14
(1,42)	1:20:A:ASP:H	1:79:A:GLN:H	8	0.14
(1,39)	1:19:A:LYS:H	1:79:A:GLN:H	18	0.14
(1,15)	1:12:A:GLN:H	1:85:A:SER:H	17	0.14
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	10	0.13
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	10	0.13
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	10	0.13
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	10	0.13
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	10	0.13
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	10	0.13
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG11	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG12	3	0.13
(1,1671)	1:86:D:ILE:HD11	2:452:H:VAL:HG13	3	0.13
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG11	3	0.13
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG12	3	0.13
(1,1671)	1:86:D:ILE:HD12	2:452:H:VAL:HG13	3	0.13
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG11	3	0.13
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG12	3	0.13
(1,1671)	1:86:D:ILE:HD13	2:452:H:VAL:HG13	3	0.13
(1,1669)	1:131:D:VAL:HG21	2:464:H:MET:HE1	6	0.13
(1,1669)	1:131:D:VAL:HG21	2:464:H:MET:HE2	6	0.13
(1,1669)	1:131:D:VAL:HG21	2:464:H:MET:HE3	6	0.13
(1,1669)	1:131:D:VAL:HG22	2:464:H:MET:HE1	6	0.13
(1,1669)	1:131:D:VAL:HG22	2:464:H:MET:HE2	6	0.13
(1,1669)	1:131:D:VAL:HG22	2:464:H:MET:HE3	6	0.13
(1,1669)	1:131:D:VAL:HG23	2:464:H:MET:HE1	6	0.13
(1,1669)	1:131:D:VAL:HG23	2:464:H:MET:HE2	6	0.13
(1,1669)	1:131:D:VAL:HG23	2:464:H:MET:HE3	6	0.13
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD1	8	0.13
(1,1655)	1:131:C:VAL:HG21	2:462:G:TYR:HD2	8	0.13
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD1	8	0.13
(1,1655)	1:131:C:VAL:HG22	2:462:G:TYR:HD2	8	0.13
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD1	8	0.13
(1,1655)	1:131:C:VAL:HG23	2:462:G:TYR:HD2	8	0.13
(1,1647)	1:86:C:ILE:HD11	2:451:G:VAL:HG11	5	0.13
(1,1647)	1:86:C:ILE:HD11	2:451:G:VAL:HG12	5	0.13
(1,1647)	1:86:C:ILE:HD11	2:451:G:VAL:HG13	5	0.13
(1,1647)	1:86:C:ILE:HD11	2:451:G:VAL:HG21	5	0.13
(1,1647)	1:86:C:ILE:HD11	2:451:G:VAL:HG22	5	0.13
(1,1647)	1:86:C:ILE:HD11	2:451:G:VAL:HG23	5	0.13
(1,1647)	1:86:C:ILE:HD12	2:451:G:VAL:HG11	5	0.13
(1,1647)	1:86:C:ILE:HD12	2:451:G:VAL:HG12	5	0.13
(1,1647)	1:86:C:ILE:HD12	2:451:G:VAL:HG13	5	0.13
(1,1647)	1:86:C:ILE:HD12	2:451:G:VAL:HG21	5	0.13
(1,1647)	1:86:C:ILE:HD12	2:451:G:VAL:HG22	5	0.13
(1,1647)	1:86:C:ILE:HD12	2:451:G:VAL:HG23	5	0.13
(1,1647)	1:86:C:ILE:HD13	2:451:G:VAL:HG11	5	0.13
(1,1647)	1:86:C:ILE:HD13	2:451:G:VAL:HG12	5	0.13
(1,1647)	1:86:C:ILE:HD13	2:451:G:VAL:HG13	5	0.13
(1,1647)	1:86:C:ILE:HD13	2:451:G:VAL:HG21	5	0.13
(1,1647)	1:86:C:ILE:HD13	2:451:G:VAL:HG22	5	0.13
(1,1647)	1:86:C:ILE:HD13	2:451:G:VAL:HG23	5	0.13
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG11	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG12	11	0.13
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG13	11	0.13
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG11	11	0.13
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG12	11	0.13
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG13	11	0.13
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG11	11	0.13
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG12	11	0.13
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG13	11	0.13
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG11	18	0.13
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG12	18	0.13
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG13	18	0.13
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG11	18	0.13
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG12	18	0.13
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG13	18	0.13
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG11	18	0.13
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG12	18	0.13
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG13	18	0.13
(1,1640)	1:36:C:TRP:HE1	2:470:G:LEU:HD11	14	0.13
(1,1640)	1:36:C:TRP:HE1	2:470:G:LEU:HD12	14	0.13
(1,1640)	1:36:C:TRP:HE1	2:470:G:LEU:HD13	14	0.13
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD11	16	0.13
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD12	16	0.13
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD13	16	0.13
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD21	16	0.13
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD22	16	0.13
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD23	16	0.13
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD11	16	0.13
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD12	16	0.13
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD13	16	0.13
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD21	16	0.13
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD22	16	0.13
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD23	16	0.13
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD11	16	0.13
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD12	16	0.13
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD13	16	0.13
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD21	16	0.13
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD22	16	0.13
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD23	16	0.13
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD11	16	0.13
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD12	16	0.13
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD13	16	0.13
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD21	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD22	16	0.13
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD23	16	0.13
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD11	16	0.13
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD12	16	0.13
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD13	16	0.13
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD21	16	0.13
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD22	16	0.13
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD23	16	0.13
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD11	16	0.13
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD12	16	0.13
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD13	16	0.13
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD21	16	0.13
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD22	16	0.13
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD23	16	0.13
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	10	0.13
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	10	0.13
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	10	0.13
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	10	0.13
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	10	0.13
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	10	0.13
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	15	0.13
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	15	0.13
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	15	0.13
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	15	0.13
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	15	0.13
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	15	0.13
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG11	17	0.13
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG12	17	0.13
(1,1622)	1:94:B:MET:HE1	2:452:F:VAL:HG13	17	0.13
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG11	17	0.13
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG12	17	0.13
(1,1622)	1:94:B:MET:HE2	2:452:F:VAL:HG13	17	0.13
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG11	17	0.13
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG12	17	0.13
(1,1622)	1:94:B:MET:HE3	2:452:F:VAL:HG13	17	0.13
(1,1616)	1:98:B:LEU:HD11	2:454:F:LEU:HD21	9	0.13
(1,1616)	1:98:B:LEU:HD11	2:454:F:LEU:HD22	9	0.13
(1,1616)	1:98:B:LEU:HD11	2:454:F:LEU:HD23	9	0.13
(1,1616)	1:98:B:LEU:HD12	2:454:F:LEU:HD21	9	0.13
(1,1616)	1:98:B:LEU:HD12	2:454:F:LEU:HD22	9	0.13
(1,1616)	1:98:B:LEU:HD12	2:454:F:LEU:HD23	9	0.13
(1,1616)	1:98:B:LEU:HD13	2:454:F:LEU:HD21	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:98:B:LEU:HD13	2:454:F:LEU:HD22	9	0.13
(1,1616)	1:98:B:LEU:HD13	2:454:F:LEU:HD23	9	0.13
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	14	0.13
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	14	0.13
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	14	0.13
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	19	0.13
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	19	0.13
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	19	0.13
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD11	17	0.13
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD12	17	0.13
(1,1611)	1:74:B:PHE:HE1	2:470:F:LEU:HD13	17	0.13
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD11	17	0.13
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD12	17	0.13
(1,1611)	1:74:B:PHE:HE2	2:470:F:LEU:HD13	17	0.13
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	17	0.13
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	17	0.13
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	17	0.13
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	17	0.13
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	17	0.13
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	17	0.13
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	17	0.13
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	17	0.13
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	17	0.13
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	17	0.13
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	17	0.13
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	17	0.13
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	17	0.13
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	17	0.13
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	17	0.13
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	17	0.13
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	17	0.13
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	17	0.13
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	17	0.13
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	17	0.13
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	17	0.13
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	17	0.13
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	17	0.13
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	17	0.13
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	17	0.13
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	17	0.13
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	17	0.13
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	17	0.13
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	17	0.13
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	17	0.13
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	17	0.13
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	17	0.13
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	17	0.13
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	17	0.13
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	17	0.13
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE1	12	0.13
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE2	12	0.13
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE3	12	0.13
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE1	12	0.13
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE2	12	0.13
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE3	12	0.13
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE1	12	0.13
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE2	12	0.13
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE3	12	0.13
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD1	14	0.13
(1,1601)	1:131:A:VAL:HG21	2:462:E:TYR:HD2	14	0.13
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD1	14	0.13
(1,1601)	1:131:A:VAL:HG22	2:462:E:TYR:HD2	14	0.13
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD1	14	0.13
(1,1601)	1:131:A:VAL:HG23	2:462:E:TYR:HD2	14	0.13
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	4	0.13
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	4	0.13
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	4	0.13
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	4	0.13
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	4	0.13
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	4	0.13
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	8	0.13
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	8	0.13
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	8	0.13
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	8	0.13
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	8	0.13
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	8	0.13
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD11	20	0.13
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD12	20	0.13
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD13	20	0.13
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD11	20	0.13
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD12	20	0.13
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD13	20	0.13
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD11	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD12	20	0.13
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD13	20	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG11	15	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG12	15	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG13	15	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG21	15	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG22	15	0.13
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG23	15	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG11	15	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG12	15	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG13	15	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG21	15	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG22	15	0.13
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG23	15	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG11	15	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG12	15	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG13	15	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG21	15	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG22	15	0.13
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG23	15	0.13
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG21	13	0.13
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG22	13	0.13
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG23	13	0.13
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG21	13	0.13
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG22	13	0.13
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG23	13	0.13
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG11	12	0.13
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG12	12	0.13
(1,1590)	1:86:A:ILE:HD11	2:452:E:VAL:HG13	12	0.13
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG11	12	0.13
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG12	12	0.13
(1,1590)	1:86:A:ILE:HD12	2:452:E:VAL:HG13	12	0.13
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG11	12	0.13
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG12	12	0.13
(1,1590)	1:86:A:ILE:HD13	2:452:E:VAL:HG13	12	0.13
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD11	9	0.13
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD12	9	0.13
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD13	9	0.13
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	7	0.13
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	10	0.13
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD11	9	0.13
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD12	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:131:D:VAL:HG11	1:136:D:LEU:HD13	9	0.13
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD11	9	0.13
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD12	9	0.13
(1,1550)	1:131:D:VAL:HG12	1:136:D:LEU:HD13	9	0.13
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD11	9	0.13
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD12	9	0.13
(1,1550)	1:131:D:VAL:HG13	1:136:D:LEU:HD13	9	0.13
(1,1543)	1:127:D:ASN:H	1:128:D:LEU:H	4	0.13
(1,1540)	1:126:D:LEU:H	1:127:D:ASN:H	7	0.13
(1,1505)	1:110:D:ALA:H	1:111:D:ARG:H	4	0.13
(1,1470)	1:93:D:GLN:H	1:96:D:HIS:H	15	0.13
(1,1464)	1:91:D:GLY:H	1:95:D:ALA:H	5	0.13
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB1	1	0.13
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB2	1	0.13
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB3	1	0.13
(1,1414)	1:68:D:LEU:H	1:71:D:GLU:H	15	0.13
(1,1387)	1:62:D:VAL:HG21	1:110:D:ALA:HB1	19	0.13
(1,1387)	1:62:D:VAL:HG21	1:110:D:ALA:HB2	19	0.13
(1,1387)	1:62:D:VAL:HG21	1:110:D:ALA:HB3	19	0.13
(1,1387)	1:62:D:VAL:HG22	1:110:D:ALA:HB1	19	0.13
(1,1387)	1:62:D:VAL:HG22	1:110:D:ALA:HB2	19	0.13
(1,1387)	1:62:D:VAL:HG22	1:110:D:ALA:HB3	19	0.13
(1,1387)	1:62:D:VAL:HG23	1:110:D:ALA:HB1	19	0.13
(1,1387)	1:62:D:VAL:HG23	1:110:D:ALA:HB2	19	0.13
(1,1387)	1:62:D:VAL:HG23	1:110:D:ALA:HB3	19	0.13
(1,1360)	1:58:D:VAL:H	1:84:D:PHE:H	19	0.13
(1,1330)	1:50:D:GLN:H	1:57:D:GLU:H	10	0.13
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	16	0.13
(1,1274)	1:36:D:TRP:HE3	1:37:D:GLN:H	9	0.13
(1,1271)	1:35:D:ASP:H	1:36:D:TRP:H	19	0.13
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	5	0.13
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	18	0.13
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	20	0.13
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	12	0.13
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	7	0.13
(1,1185)	1:136:C:LEU:H	1:138:C:MET:H	16	0.13
(1,1175)	1:133:C:PHE:H	1:136:C:LEU:H	1	0.13
(1,1174)	1:133:C:PHE:H	1:135:C:ALA:H	1	0.13
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	5	0.13
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	6	0.13
(1,1173)	1:133:C:PHE:H	1:134:C:ASP:H	17	0.13
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	13	0.13
(1,1125)	1:110:C:ALA:H	1:111:C:ARG:H	10	0.13
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	18	0.13
(1,1055)	1:77:C:GLU:H	1:78:C:VAL:H	20	0.13
(1,1027)	1:68:C:LEU:H	1:69:C:GLY:H	7	0.13
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD11	8	0.13
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD12	8	0.13
(1,1008)	1:64:C:VAL:HG11	1:126:C:LEU:HD13	8	0.13
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD11	8	0.13
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD12	8	0.13
(1,1008)	1:64:C:VAL:HG12	1:126:C:LEU:HD13	8	0.13
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD11	8	0.13
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD12	8	0.13
(1,1008)	1:64:C:VAL:HG13	1:126:C:LEU:HD13	8	0.13
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD11	9	0.13
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD12	9	0.13
(1,1000)	1:62:C:VAL:HG11	1:128:C:LEU:HD13	9	0.13
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD11	9	0.13
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD12	9	0.13
(1,1000)	1:62:C:VAL:HG12	1:128:C:LEU:HD13	9	0.13
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD11	9	0.13
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD12	9	0.13
(1,1000)	1:62:C:VAL:HG13	1:128:C:LEU:HD13	9	0.13
(1,995)	1:62:C:VAL:H	1:63:C:THR:H	5	0.13
(1,969)	1:56:C:TYR:HD1	1:98:C:LEU:HD21	1	0.13
(1,969)	1:56:C:TYR:HD1	1:98:C:LEU:HD22	1	0.13
(1,969)	1:56:C:TYR:HD1	1:98:C:LEU:HD23	1	0.13
(1,969)	1:56:C:TYR:HD2	1:98:C:LEU:HD21	1	0.13
(1,969)	1:56:C:TYR:HD2	1:98:C:LEU:HD22	1	0.13
(1,969)	1:56:C:TYR:HD2	1:98:C:LEU:HD23	1	0.13
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	9	0.13
(1,941)	1:51:C:LEU:H	1:52:C:ALA:H	2	0.13
(1,941)	1:51:C:LEU:H	1:52:C:ALA:H	12	0.13
(1,940)	1:50:C:GLN:H	1:57:C:GLU:H	14	0.13
(1,936)	1:49:C:SER:H	1:59:C:VAL:H	16	0.13
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	20	0.13
(1,932)	1:48:C:SER:H	1:59:C:VAL:H	13	0.13
(1,901)	1:42:C:LEU:H	1:65:C:THR:H	11	0.13
(1,899)	1:41:C:LYS:H	1:67:C:SER:H	6	0.13
(1,892)	1:40:C:VAL:HG21	1:41:C:LYS:H	5	0.13
(1,892)	1:40:C:VAL:HG22	1:41:C:LYS:H	5	0.13
(1,892)	1:40:C:VAL:HG23	1:41:C:LYS:H	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,855)	1:25:C:ALA:H	1:21:D:ILE:H	20	0.13
(1,844)	1:22:C:SER:H	1:23:D:PHE:H	16	0.13
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	9	0.13
(1,754)	1:126:B:LEU:H	1:127:B:ASN:H	6	0.13
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	3	0.13
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	12	0.13
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	15	0.13
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	19	0.13
(1,713)	1:101:B:TYR:H	1:102:B:CYS:H	16	0.13
(1,704)	1:99:B:GLY:H	1:100:B:ALA:H	10	0.13
(1,689)	1:95:B:ALA:H	1:98:B:LEU:H	17	0.13
(1,679)	1:92:B:THR:H	1:94:B:MET:H	14	0.13
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	14	0.13
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	10	0.13
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	10	0.13
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	17	0.13
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	13	0.13
(1,622)	1:68:B:LEU:H	1:71:B:GLU:H	4	0.13
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	2	0.13
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	4	0.13
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	12	0.13
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	7	0.13
(1,528)	1:48:B:SER:H	1:59:B:VAL:H	7	0.13
(1,524)	1:47:B:ALA:H	1:61:B:ARG:H	19	0.13
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	6	0.13
(1,516)	1:45:B:ASP:H	1:46:B:THR:H	9	0.13
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG21	5	0.13
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG22	5	0.13
(1,499)	1:42:B:LEU:HD11	1:64:B:VAL:HG23	5	0.13
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG21	5	0.13
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG22	5	0.13
(1,499)	1:42:B:LEU:HD12	1:64:B:VAL:HG23	5	0.13
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG21	5	0.13
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG22	5	0.13
(1,499)	1:42:B:LEU:HD13	1:64:B:VAL:HG23	5	0.13
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG11	8	0.13
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG12	8	0.13
(1,498)	1:42:B:LEU:HD11	1:62:B:VAL:HG13	8	0.13
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG11	8	0.13
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG12	8	0.13
(1,498)	1:42:B:LEU:HD12	1:62:B:VAL:HG13	8	0.13
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG11	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG12	8	0.13
(1,498)	1:42:B:LEU:HD13	1:62:B:VAL:HG13	8	0.13
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	2	0.13
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	2	0.13
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	2	0.13
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	2	0.13
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	2	0.13
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	2	0.13
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	2	0.13
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	2	0.13
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	2	0.13
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	9	0.13
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	9	0.13
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	9	0.13
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	9	0.13
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	9	0.13
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	9	0.13
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	9	0.13
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	9	0.13
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	9	0.13
(1,451)	1:30:B:HIS:H	1:32:B:PHE:H	18	0.13
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB1	1	0.13
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB2	1	0.13
(1,446)	1:25:B:ALA:HB1	1:28:B:ALA:HB3	1	0.13
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB1	1	0.13
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB2	1	0.13
(1,446)	1:25:B:ALA:HB2	1:28:B:ALA:HB3	1	0.13
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB1	1	0.13
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB2	1	0.13
(1,446)	1:25:B:ALA:HB3	1:28:B:ALA:HB3	1	0.13
(1,410)	1:12:B:GLN:H	1:13:B:ILE:H	16	0.13
(1,395)	1:140:A:TYR:H	1:141:A:LEU:H	5	0.13
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	19	0.13
(1,359)	1:122:A:THR:H	1:18:B:THR:H	4	0.13
(1,359)	1:122:A:THR:H	1:18:B:THR:H	13	0.13
(1,356)	1:121:A:GLY:H	1:123:A:PHE:H	7	0.13
(1,354)	1:119:A:SER:H	1:123:A:PHE:H	5	0.13
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	12	0.13
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	20	0.13
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	1	0.13
(1,306)	1:99:A:GLY:H	1:100:A:ALA:H	15	0.13
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	3	0.13
(1,293)	1:96:A:HIS:H	1:97:A:CYS:H	1	0.13
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE1	18	0.13
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE2	18	0.13
(1,277)	1:91:A:GLY:H	1:94:A:MET:HE3	18	0.13
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	3	0.13
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	19	0.13
(1,180)	1:59:A:VAL:HG21	1:82:A:GLY:H	19	0.13
(1,180)	1:59:A:VAL:HG22	1:82:A:GLY:H	19	0.13
(1,180)	1:59:A:VAL:HG23	1:82:A:GLY:H	19	0.13
(1,179)	1:59:A:VAL:HG21	1:81:A:GLY:H	6	0.13
(1,179)	1:59:A:VAL:HG22	1:81:A:GLY:H	6	0.13
(1,179)	1:59:A:VAL:HG23	1:81:A:GLY:H	6	0.13
(1,176)	1:59:A:VAL:HG11	1:80:A:GLN:H	19	0.13
(1,176)	1:59:A:VAL:HG12	1:80:A:GLN:H	19	0.13
(1,176)	1:59:A:VAL:HG13	1:80:A:GLN:H	19	0.13
(1,158)	1:55:A:VAL:H	1:56:A:TYR:H	10	0.13
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE1	2	0.13
(1,157)	1:54:A:ASP:H	1:56:A:TYR:HE2	2	0.13
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	12	0.13
(1,140)	1:51:A:LEU:H	1:52:A:ALA:H	19	0.13
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	13	0.13
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD11	16	0.13
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD12	16	0.13
(1,93)	1:37:A:GLN:H	1:68:A:LEU:HD13	16	0.13
(1,82)	1:33:A:GLN:H	1:34:A:LYS:H	6	0.13
(1,50)	1:22:A:SER:H	1:79:A:GLN:H	3	0.13
(1,50)	1:22:A:SER:H	1:79:A:GLN:H	11	0.13
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	1	0.13
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	6	0.13
(1,21)	1:14:A:GLN:H	1:85:A:SER:H	8	0.13
(1,19)	1:14:A:GLN:H	1:84:A:PHE:H	2	0.13
(1,1688)	1:126:D:LEU:HD11	2:468:H:LEU:HD11	1	0.12
(1,1688)	1:126:D:LEU:HD11	2:468:H:LEU:HD12	1	0.12
(1,1688)	1:126:D:LEU:HD11	2:468:H:LEU:HD13	1	0.12
(1,1688)	1:126:D:LEU:HD11	2:468:H:LEU:HD21	1	0.12
(1,1688)	1:126:D:LEU:HD11	2:468:H:LEU:HD22	1	0.12
(1,1688)	1:126:D:LEU:HD11	2:468:H:LEU:HD23	1	0.12
(1,1688)	1:126:D:LEU:HD12	2:468:H:LEU:HD11	1	0.12
(1,1688)	1:126:D:LEU:HD12	2:468:H:LEU:HD12	1	0.12
(1,1688)	1:126:D:LEU:HD12	2:468:H:LEU:HD13	1	0.12
(1,1688)	1:126:D:LEU:HD12	2:468:H:LEU:HD21	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:126:D:LEU:HD12	2:468:H:LEU:HD22	1	0.12
(1,1688)	1:126:D:LEU:HD12	2:468:H:LEU:HD23	1	0.12
(1,1688)	1:126:D:LEU:HD13	2:468:H:LEU:HD11	1	0.12
(1,1688)	1:126:D:LEU:HD13	2:468:H:LEU:HD12	1	0.12
(1,1688)	1:126:D:LEU:HD13	2:468:H:LEU:HD13	1	0.12
(1,1688)	1:126:D:LEU:HD13	2:468:H:LEU:HD21	1	0.12
(1,1688)	1:126:D:LEU:HD13	2:468:H:LEU:HD22	1	0.12
(1,1688)	1:126:D:LEU:HD13	2:468:H:LEU:HD23	1	0.12
(1,1688)	1:126:D:LEU:HD21	2:468:H:LEU:HD11	1	0.12
(1,1688)	1:126:D:LEU:HD21	2:468:H:LEU:HD12	1	0.12
(1,1688)	1:126:D:LEU:HD21	2:468:H:LEU:HD13	1	0.12
(1,1688)	1:126:D:LEU:HD21	2:468:H:LEU:HD21	1	0.12
(1,1688)	1:126:D:LEU:HD21	2:468:H:LEU:HD22	1	0.12
(1,1688)	1:126:D:LEU:HD21	2:468:H:LEU:HD23	1	0.12
(1,1688)	1:126:D:LEU:HD22	2:468:H:LEU:HD11	1	0.12
(1,1688)	1:126:D:LEU:HD22	2:468:H:LEU:HD12	1	0.12
(1,1688)	1:126:D:LEU:HD22	2:468:H:LEU:HD13	1	0.12
(1,1688)	1:126:D:LEU:HD22	2:468:H:LEU:HD21	1	0.12
(1,1688)	1:126:D:LEU:HD22	2:468:H:LEU:HD22	1	0.12
(1,1688)	1:126:D:LEU:HD22	2:468:H:LEU:HD23	1	0.12
(1,1688)	1:126:D:LEU:HD23	2:468:H:LEU:HD11	1	0.12
(1,1688)	1:126:D:LEU:HD23	2:468:H:LEU:HD12	1	0.12
(1,1688)	1:126:D:LEU:HD23	2:468:H:LEU:HD13	1	0.12
(1,1688)	1:126:D:LEU:HD23	2:468:H:LEU:HD21	1	0.12
(1,1688)	1:126:D:LEU:HD23	2:468:H:LEU:HD22	1	0.12
(1,1688)	1:126:D:LEU:HD23	2:468:H:LEU:HD23	1	0.12
(1,1681)	1:131:D:VAL:HG11	2:462:H:TYR:HD1	12	0.12
(1,1681)	1:131:D:VAL:HG11	2:462:H:TYR:HD2	12	0.12
(1,1681)	1:131:D:VAL:HG12	2:462:H:TYR:HD1	12	0.12
(1,1681)	1:131:D:VAL:HG12	2:462:H:TYR:HD2	12	0.12
(1,1681)	1:131:D:VAL:HG13	2:462:H:TYR:HD1	12	0.12
(1,1681)	1:131:D:VAL:HG13	2:462:H:TYR:HD2	12	0.12
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG11	13	0.12
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG12	13	0.12
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG13	13	0.12
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG11	13	0.12
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG12	13	0.12
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG13	13	0.12
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG11	13	0.12
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG12	13	0.12
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG13	13	0.12
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	5	0.12
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	5	0.12
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD11	6	0.12
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD12	6	0.12
(1,1663)	1:74:D:PHE:HZ	2:468:H:LEU:HD13	6	0.12
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE1	17	0.12
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE2	17	0.12
(1,1656)	1:42:C:LEU:HD21	2:464:G:MET:HE3	17	0.12
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE1	17	0.12
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE2	17	0.12
(1,1656)	1:42:C:LEU:HD22	2:464:G:MET:HE3	17	0.12
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE1	17	0.12
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE2	17	0.12
(1,1656)	1:42:C:LEU:HD23	2:464:G:MET:HE3	17	0.12
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD11	2	0.12
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD12	2	0.12
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD13	2	0.12
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD11	2	0.12
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD12	2	0.12
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD13	2	0.12
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD11	13	0.12
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD12	13	0.12
(1,1650)	1:44:C:LEU:HD11	2:460:G:LEU:HD13	13	0.12
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD11	13	0.12
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD12	13	0.12
(1,1650)	1:44:C:LEU:HD12	2:460:G:LEU:HD13	13	0.12
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD11	13	0.12
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD12	13	0.12
(1,1650)	1:44:C:LEU:HD13	2:460:G:LEU:HD13	13	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG21	11	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG22	11	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG23	11	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG21	11	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG22	11	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG23	11	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG21	14	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG22	14	0.12
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG23	14	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG21	14	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG22	14	0.12
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG23	14	0.12
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG11	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG12	17	0.12
(1,1644)	1:86:C:ILE:HD11	2:452:G:VAL:HG13	17	0.12
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG11	17	0.12
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG12	17	0.12
(1,1644)	1:86:C:ILE:HD12	2:452:G:VAL:HG13	17	0.12
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG11	17	0.12
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG12	17	0.12
(1,1644)	1:86:C:ILE:HD13	2:452:G:VAL:HG13	17	0.12
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD21	1	0.12
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD22	1	0.12
(1,1643)	1:98:C:LEU:HD11	2:454:G:LEU:HD23	1	0.12
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD21	1	0.12
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD22	1	0.12
(1,1643)	1:98:C:LEU:HD12	2:454:G:LEU:HD23	1	0.12
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD21	1	0.12
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD22	1	0.12
(1,1643)	1:98:C:LEU:HD13	2:454:G:LEU:HD23	1	0.12
(1,1633)	1:40:B:VAL:HG11	2:468:F:LEU:HD11	3	0.12
(1,1633)	1:40:B:VAL:HG11	2:468:F:LEU:HD12	3	0.12
(1,1633)	1:40:B:VAL:HG11	2:468:F:LEU:HD13	3	0.12
(1,1633)	1:40:B:VAL:HG12	2:468:F:LEU:HD11	3	0.12
(1,1633)	1:40:B:VAL:HG12	2:468:F:LEU:HD12	3	0.12
(1,1633)	1:40:B:VAL:HG12	2:468:F:LEU:HD13	3	0.12
(1,1633)	1:40:B:VAL:HG13	2:468:F:LEU:HD11	3	0.12
(1,1633)	1:40:B:VAL:HG13	2:468:F:LEU:HD12	3	0.12
(1,1633)	1:40:B:VAL:HG13	2:468:F:LEU:HD13	3	0.12
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB1	17	0.12
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB2	17	0.12
(1,1631)	1:40:B:VAL:HG11	2:467:F:ALA:HB3	17	0.12
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB1	17	0.12
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB2	17	0.12
(1,1631)	1:40:B:VAL:HG12	2:467:F:ALA:HB3	17	0.12
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB1	17	0.12
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB2	17	0.12
(1,1631)	1:40:B:VAL:HG13	2:467:F:ALA:HB3	17	0.12
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB1	17	0.12
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB2	17	0.12
(1,1631)	1:40:B:VAL:HG21	2:467:F:ALA:HB3	17	0.12
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB1	17	0.12
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB2	17	0.12
(1,1631)	1:40:B:VAL:HG22	2:467:F:ALA:HB3	17	0.12
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB1	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB2	17	0.12
(1,1631)	1:40:B:VAL:HG23	2:467:F:ALA:HB3	17	0.12
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	2	0.12
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	2	0.12
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	2	0.12
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	2	0.12
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	2	0.12
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	2	0.12
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	3	0.12
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	3	0.12
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	3	0.12
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	3	0.12
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	3	0.12
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	3	0.12
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE1	20	0.12
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE2	20	0.12
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE1	20	0.12
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE2	20	0.12
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE1	20	0.12
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE2	20	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	12	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	12	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	12	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	12	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	12	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	12	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	12	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	12	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	12	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	12	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	12	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	12	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	12	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	12	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	12	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	12	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	12	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	12	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	12	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	12	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	12	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	12	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	12	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	12	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	12	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	12	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	12	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	12	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	12	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	12	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	12	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	12	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	12	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	12	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	12	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD11	16	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD12	16	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD13	16	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD21	16	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD22	16	0.12
(1,1605)	1:58:A:VAL:HG11	2:454:E:LEU:HD23	16	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD11	16	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD12	16	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD13	16	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD21	16	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD22	16	0.12
(1,1605)	1:58:A:VAL:HG12	2:454:E:LEU:HD23	16	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD11	16	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD12	16	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD13	16	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD21	16	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD22	16	0.12
(1,1605)	1:58:A:VAL:HG13	2:454:E:LEU:HD23	16	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD11	16	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD12	16	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD13	16	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD21	16	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD22	16	0.12
(1,1605)	1:58:A:VAL:HG21	2:454:E:LEU:HD23	16	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD11	16	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD12	16	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD13	16	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD21	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD22	16	0.12
(1,1605)	1:58:A:VAL:HG22	2:454:E:LEU:HD23	16	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD11	16	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD12	16	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD13	16	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD21	16	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD22	16	0.12
(1,1605)	1:58:A:VAL:HG23	2:454:E:LEU:HD23	16	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB1	12	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB2	12	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB3	12	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB1	12	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB2	12	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB3	12	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB1	12	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB2	12	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB3	12	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB1	12	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB2	12	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB3	12	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB1	12	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB2	12	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB3	12	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB1	12	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB2	12	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB3	12	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB1	17	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB2	17	0.12
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB3	17	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB1	17	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB2	17	0.12
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB3	17	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB1	17	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB2	17	0.12
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB3	17	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB1	17	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB2	17	0.12
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB3	17	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB1	17	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB2	17	0.12
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB3	17	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB1	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB2	17	0.12
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB3	17	0.12
(1,1599)	1:100:A:ALA:HB1	2:461:E:PHE:HZ	17	0.12
(1,1599)	1:100:A:ALA:HB2	2:461:E:PHE:HZ	17	0.12
(1,1599)	1:100:A:ALA:HB3	2:461:E:PHE:HZ	17	0.12
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE1	19	0.12
(1,1598)	1:136:A:LEU:HD21	2:461:E:PHE:HE2	19	0.12
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE1	19	0.12
(1,1598)	1:136:A:LEU:HD22	2:461:E:PHE:HE2	19	0.12
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE1	19	0.12
(1,1598)	1:136:A:LEU:HD23	2:461:E:PHE:HE2	19	0.12
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD11	14	0.12
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD12	14	0.12
(1,1596)	1:44:A:LEU:HD11	2:460:E:LEU:HD13	14	0.12
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD11	14	0.12
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD12	14	0.12
(1,1596)	1:44:A:LEU:HD12	2:460:E:LEU:HD13	14	0.12
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD11	14	0.12
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD12	14	0.12
(1,1596)	1:44:A:LEU:HD13	2:460:E:LEU:HD13	14	0.12
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG11	12	0.12
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG12	12	0.12
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG13	12	0.12
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG21	12	0.12
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG22	12	0.12
(1,1593)	1:86:A:ILE:HD11	2:451:E:VAL:HG23	12	0.12
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG11	12	0.12
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG12	12	0.12
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG13	12	0.12
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG21	12	0.12
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG22	12	0.12
(1,1593)	1:86:A:ILE:HD12	2:451:E:VAL:HG23	12	0.12
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG11	12	0.12
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG12	12	0.12
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG13	12	0.12
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG21	12	0.12
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG22	12	0.12
(1,1593)	1:86:A:ILE:HD13	2:451:E:VAL:HG23	12	0.12
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD11	16	0.12
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD12	16	0.12
(1,1586)	1:36:A:TRP:HE1	2:470:E:LEU:HD13	16	0.12
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD11	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD12	1	0.12
(1,1582)	1:74:A:PHE:HZ	2:468:E:LEU:HD13	1	0.12
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	18	0.12
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	1	0.12
(1,1551)	1:133:D:PHE:H	1:134:D:ASP:H	3	0.12
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG21	20	0.12
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG22	20	0.12
(1,1547)	1:128:D:LEU:HD21	1:131:D:VAL:HG23	20	0.12
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG21	20	0.12
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG22	20	0.12
(1,1547)	1:128:D:LEU:HD22	1:131:D:VAL:HG23	20	0.12
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG21	20	0.12
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG22	20	0.12
(1,1547)	1:128:D:LEU:HD23	1:131:D:VAL:HG23	20	0.12
(1,1540)	1:126:D:LEU:H	1:127:D:ASN:H	9	0.12
(1,1506)	1:110:D:ALA:H	1:112:D:GLU:H	16	0.12
(1,1490)	1:99:D:GLY:H	1:100:D:ALA:H	17	0.12
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	9	0.12
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	17	0.12
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB1	12	0.12
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB2	12	0.12
(1,1447)	1:80:D:GLN:H	1:110:D:ALA:HB3	12	0.12
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	8	0.12
(1,1372)	1:60:D:LEU:H	1:82:D:GLY:H	9	0.12
(1,1345)	1:54:D:ASP:H	1:55:D:VAL:H	1	0.12
(1,1271)	1:35:D:ASP:H	1:36:D:TRP:H	12	0.12
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	15	0.12
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	20	0.12
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	12	0.12
(1,1210)	1:14:D:GLN:H	1:15:D:ARG:H	17	0.12
(1,1208)	1:12:D:GLN:H	1:85:D:SER:H	14	0.12
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	13	0.12
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	12	0.12
(1,1112)	1:99:C:GLY:H	1:102:C:CYS:H	1	0.12
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	14	0.12
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	14	0.12
(1,1103)	1:97:C:CYS:H	1:100:C:ALA:H	15	0.12
(1,1094)	1:95:C:ALA:H	1:98:C:LEU:H	18	0.12
(1,1092)	1:95:C:ALA:H	1:96:C:HIS:H	4	0.12
(1,1073)	1:87:C:ALA:H	1:88:C:GLY:H	11	0.12
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	19	0.12
(1,995)	1:62:C:VAL:H	1:63:C:THR:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:62:C:VAL:H	1:63:C:THR:H	15	0.12
(1,985)	1:60:C:LEU:H	1:81:C:GLY:H	4	0.12
(1,972)	1:58:C:VAL:H	1:59:C:VAL:H	3	0.12
(1,935)	1:49:C:SER:H	1:58:C:VAL:H	4	0.12
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	15	0.12
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	19	0.12
(1,844)	1:22:C:SER:H	1:23:D:PHE:H	12	0.12
(1,841)	1:22:C:SER:H	1:78:C:VAL:H	10	0.12
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	7	0.12
(1,806)	1:12:C:GLN:H	1:13:C:ILE:H	20	0.12
(1,720)	1:110:B:ALA:H	1:112:B:GLU:H	8	0.12
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	10	0.12
(1,715)	1:109:B:TYR:H	1:110:B:ALA:H	3	0.12
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	20	0.12
(1,694)	1:96:B:HIS:H	1:99:B:GLY:H	18	0.12
(1,693)	1:96:B:HIS:H	1:98:B:LEU:H	8	0.12
(1,685)	1:94:B:MET:H	1:97:B:CYS:H	16	0.12
(1,678)	1:92:B:THR:H	1:93:B:GLN:H	11	0.12
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	5	0.12
(1,670)	1:88:B:GLY:H	1:89:B:ILE:H	13	0.12
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	19	0.12
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	19	0.12
(1,624)	1:68:B:LEU:H	1:73:B:ALA:H	2	0.12
(1,621)	1:68:B:LEU:H	1:69:B:GLY:H	2	0.12
(1,621)	1:68:B:LEU:H	1:69:B:GLY:H	14	0.12
(1,620)	1:67:B:SER:H	1:74:B:PHE:H	7	0.12
(1,607)	1:66:B:ALA:H	1:73:B:ALA:H	10	0.12
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	1	0.12
(1,577)	1:60:B:LEU:H	1:82:B:GLY:H	4	0.12
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD21	5	0.12
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD22	5	0.12
(1,559)	1:56:B:TYR:HD1	1:98:B:LEU:HD23	5	0.12
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD21	5	0.12
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD22	5	0.12
(1,559)	1:56:B:TYR:HD2	1:98:B:LEU:HD23	5	0.12
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	19	0.12
(1,535)	1:51:B:LEU:H	1:52:B:ALA:H	17	0.12
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	15	0.12
(1,534)	1:50:B:GLN:H	1:57:B:GLU:H	18	0.12
(1,533)	1:50:B:GLN:H	1:51:B:LEU:H	9	0.12
(1,528)	1:48:B:SER:H	1:59:B:VAL:H	3	0.12
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:47:B:ALA:H	1:59:B:VAL:H	11	0.12
(1,522)	1:47:B:ALA:H	1:48:B:SER:H	6	0.12
(1,522)	1:47:B:ALA:H	1:48:B:SER:H	17	0.12
(1,473)	1:36:B:TRP:HE3	1:37:B:GLN:H	20	0.12
(1,465)	1:32:B:PHE:H	1:34:B:LYS:H	11	0.12
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	20	0.12
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	20	0.12
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	20	0.12
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	20	0.12
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	20	0.12
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	20	0.12
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	20	0.12
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	20	0.12
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	20	0.12
(1,449)	1:28:B:ALA:H	1:31:B:VAL:H	4	0.12
(1,449)	1:28:B:ALA:H	1:31:B:VAL:H	16	0.12
(1,410)	1:12:B:GLN:H	1:13:B:ILE:H	10	0.12
(1,410)	1:12:B:GLN:H	1:13:B:ILE:H	11	0.12
(1,379)	1:135:A:ALA:H	1:138:A:MET:H	12	0.12
(1,366)	1:131:A:VAL:H	1:133:A:PHE:H	2	0.12
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	6	0.12
(1,359)	1:122:A:THR:H	1:18:B:THR:H	15	0.12
(1,338)	1:115:A:THR:H	1:118:A:VAL:H	20	0.12
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	4	0.12
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	6	0.12
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	8	0.12
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	16	0.12
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	18	0.12
(1,311)	1:100:A:ALA:H	1:102:A:CYS:H	16	0.12
(1,309)	1:99:A:GLY:H	1:102:A:CYS:H	16	0.12
(1,308)	1:99:A:GLY:H	1:101:A:TYR:H	20	0.12
(1,294)	1:96:A:HIS:H	1:98:A:LEU:H	7	0.12
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD21	17	0.12
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD22	17	0.12
(1,290)	1:95:A:ALA:H	1:98:A:LEU:HD23	17	0.12
(1,269)	1:87:A:ALA:H	1:89:A:ILE:H	2	0.12
(1,268)	1:87:A:ALA:H	1:88:A:GLY:H	8	0.12
(1,266)	1:85:A:SER:H	1:86:A:ILE:H	14	0.12
(1,266)	1:85:A:SER:H	1:86:A:ILE:H	18	0.12
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	20	0.12
(1,224)	1:68:A:LEU:H	1:71:A:GLU:H	2	0.12
(1,182)	1:60:A:LEU:H	1:80:A:GLN:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:59:A:VAL:HG21	1:81:A:GLY:H	17	0.12
(1,179)	1:59:A:VAL:HG22	1:81:A:GLY:H	17	0.12
(1,179)	1:59:A:VAL:HG23	1:81:A:GLY:H	17	0.12
(1,179)	1:59:A:VAL:HG21	1:81:A:GLY:H	19	0.12
(1,179)	1:59:A:VAL:HG22	1:81:A:GLY:H	19	0.12
(1,179)	1:59:A:VAL:HG23	1:81:A:GLY:H	19	0.12
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE1	18	0.12
(1,160)	1:55:A:VAL:H	1:56:A:TYR:HE2	18	0.12
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	13	0.12
(1,139)	1:50:A:GLN:H	1:57:A:GLU:H	20	0.12
(1,131)	1:47:A:ALA:H	1:61:A:ARG:H	3	0.12
(1,131)	1:47:A:ALA:H	1:61:A:ARG:H	12	0.12
(1,66)	1:28:A:ALA:H	1:30:A:HIS:H	16	0.12
(1,43)	1:21:A:ILE:H	1:22:A:SER:H	7	0.12
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	4	0.12
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	14	0.12
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD11	1	0.11
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD12	1	0.11
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD13	1	0.11
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD21	1	0.11
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD22	1	0.11
(1,1686)	1:58:D:VAL:HG11	2:454:H:LEU:HD23	1	0.11
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD11	1	0.11
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD12	1	0.11
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD13	1	0.11
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD21	1	0.11
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD22	1	0.11
(1,1686)	1:58:D:VAL:HG12	2:454:H:LEU:HD23	1	0.11
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD11	1	0.11
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD12	1	0.11
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD13	1	0.11
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD21	1	0.11
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD22	1	0.11
(1,1686)	1:58:D:VAL:HG13	2:454:H:LEU:HD23	1	0.11
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD11	1	0.11
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD12	1	0.11
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD13	1	0.11
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD21	1	0.11
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD22	1	0.11
(1,1686)	1:58:D:VAL:HG21	2:454:H:LEU:HD23	1	0.11
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD11	1	0.11
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD12	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD13	1	0.11
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD21	1	0.11
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD22	1	0.11
(1,1686)	1:58:D:VAL:HG22	2:454:H:LEU:HD23	1	0.11
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD11	1	0.11
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD12	1	0.11
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD13	1	0.11
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD21	1	0.11
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD22	1	0.11
(1,1686)	1:58:D:VAL:HG23	2:454:H:LEU:HD23	1	0.11
(1,1682)	1:131:D:VAL:HG21	2:462:H:TYR:HD1	16	0.11
(1,1682)	1:131:D:VAL:HG21	2:462:H:TYR:HD2	16	0.11
(1,1682)	1:131:D:VAL:HG22	2:462:H:TYR:HD1	16	0.11
(1,1682)	1:131:D:VAL:HG22	2:462:H:TYR:HD2	16	0.11
(1,1682)	1:131:D:VAL:HG23	2:462:H:TYR:HD1	16	0.11
(1,1682)	1:131:D:VAL:HG23	2:462:H:TYR:HD2	16	0.11
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	11	0.11
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	11	0.11
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	11	0.11
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	11	0.11
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	11	0.11
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	11	0.11
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	20	0.11
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	20	0.11
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	20	0.11
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	20	0.11
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	20	0.11
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	20	0.11
(1,1668)	1:129:D:ALA:HB1	2:464:H:MET:HE1	13	0.11
(1,1668)	1:129:D:ALA:HB1	2:464:H:MET:HE2	13	0.11
(1,1668)	1:129:D:ALA:HB1	2:464:H:MET:HE3	13	0.11
(1,1668)	1:129:D:ALA:HB2	2:464:H:MET:HE1	13	0.11
(1,1668)	1:129:D:ALA:HB2	2:464:H:MET:HE2	13	0.11
(1,1668)	1:129:D:ALA:HB2	2:464:H:MET:HE3	13	0.11
(1,1668)	1:129:D:ALA:HB3	2:464:H:MET:HE1	13	0.11
(1,1668)	1:129:D:ALA:HB3	2:464:H:MET:HE2	13	0.11
(1,1668)	1:129:D:ALA:HB3	2:464:H:MET:HE3	13	0.11
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	6	0.11
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	6	0.11
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	6	0.11
(1,1660)	1:40:C:VAL:HG11	2:468:G:LEU:HD11	10	0.11
(1,1660)	1:40:C:VAL:HG11	2:468:G:LEU:HD12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	1:40:C:VAL:HG11	2:468:G:LEU:HD13	10	0.11
(1,1660)	1:40:C:VAL:HG12	2:468:G:LEU:HD11	10	0.11
(1,1660)	1:40:C:VAL:HG12	2:468:G:LEU:HD12	10	0.11
(1,1660)	1:40:C:VAL:HG12	2:468:G:LEU:HD13	10	0.11
(1,1660)	1:40:C:VAL:HG13	2:468:G:LEU:HD11	10	0.11
(1,1660)	1:40:C:VAL:HG13	2:468:G:LEU:HD12	10	0.11
(1,1660)	1:40:C:VAL:HG13	2:468:G:LEU:HD13	10	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD11	2	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD12	2	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD13	2	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD21	2	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD22	2	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD23	2	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD11	2	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD12	2	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD13	2	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD21	2	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD22	2	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD23	2	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD11	2	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD12	2	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD13	2	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD21	2	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD22	2	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD23	2	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD11	2	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD12	2	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD13	2	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD21	2	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD22	2	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD23	2	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD11	2	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD12	2	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD13	2	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD21	2	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD22	2	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD23	2	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD11	2	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD12	2	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD13	2	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD21	2	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD22	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD23	2	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD11	12	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD12	12	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD13	12	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD21	12	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD22	12	0.11
(1,1659)	1:58:C:VAL:HG11	2:454:G:LEU:HD23	12	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD11	12	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD12	12	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD13	12	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD21	12	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD22	12	0.11
(1,1659)	1:58:C:VAL:HG12	2:454:G:LEU:HD23	12	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD11	12	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD12	12	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD13	12	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD21	12	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD22	12	0.11
(1,1659)	1:58:C:VAL:HG13	2:454:G:LEU:HD23	12	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD11	12	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD12	12	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD13	12	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD21	12	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD22	12	0.11
(1,1659)	1:58:C:VAL:HG21	2:454:G:LEU:HD23	12	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD11	12	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD12	12	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD13	12	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD21	12	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD22	12	0.11
(1,1659)	1:58:C:VAL:HG22	2:454:G:LEU:HD23	12	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD11	12	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD12	12	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD13	12	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD21	12	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD22	12	0.11
(1,1659)	1:58:C:VAL:HG23	2:454:G:LEU:HD23	12	0.11
(1,1654)	1:131:C:VAL:HG11	2:462:G:TYR:HD1	2	0.11
(1,1654)	1:131:C:VAL:HG11	2:462:G:TYR:HD2	2	0.11
(1,1654)	1:131:C:VAL:HG12	2:462:G:TYR:HD1	2	0.11
(1,1654)	1:131:C:VAL:HG12	2:462:G:TYR:HD2	2	0.11
(1,1654)	1:131:C:VAL:HG13	2:462:G:TYR:HD1	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:131:C:VAL:HG13	2:462:G:TYR:HD2	2	0.11
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE1	19	0.11
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE2	19	0.11
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE1	19	0.11
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE2	19	0.11
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE1	19	0.11
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE2	19	0.11
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG21	3	0.11
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG22	3	0.11
(1,1645)	1:56:C:TYR:HE1	2:452:G:VAL:HG23	3	0.11
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG21	3	0.11
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG22	3	0.11
(1,1645)	1:56:C:TYR:HE2	2:452:G:VAL:HG23	3	0.11
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD11	3	0.11
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD12	3	0.11
(1,1636)	1:74:C:PHE:HZ	2:468:G:LEU:HD13	3	0.11
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD11	3	0.11
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD12	3	0.11
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD13	3	0.11
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD21	3	0.11
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD22	3	0.11
(1,1635)	1:98:B:LEU:HD11	2:454:F:LEU:HD23	3	0.11
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD11	3	0.11
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD12	3	0.11
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD13	3	0.11
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD21	3	0.11
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD22	3	0.11
(1,1635)	1:98:B:LEU:HD12	2:454:F:LEU:HD23	3	0.11
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD11	3	0.11
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD12	3	0.11
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD13	3	0.11
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD21	3	0.11
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD22	3	0.11
(1,1635)	1:98:B:LEU:HD13	2:454:F:LEU:HD23	3	0.11
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD11	3	0.11
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD12	3	0.11
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD13	3	0.11
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD21	3	0.11
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD22	3	0.11
(1,1635)	1:98:B:LEU:HD21	2:454:F:LEU:HD23	3	0.11
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD11	3	0.11
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD12	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD13	3	0.11
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD21	3	0.11
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD22	3	0.11
(1,1635)	1:98:B:LEU:HD22	2:454:F:LEU:HD23	3	0.11
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD11	3	0.11
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD12	3	0.11
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD13	3	0.11
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD21	3	0.11
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD22	3	0.11
(1,1635)	1:98:B:LEU:HD23	2:454:F:LEU:HD23	3	0.11
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD11	9	0.11
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD12	9	0.11
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD13	9	0.11
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD21	9	0.11
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD22	9	0.11
(1,1632)	1:58:B:VAL:HG11	2:454:F:LEU:HD23	9	0.11
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD11	9	0.11
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD12	9	0.11
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD13	9	0.11
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD21	9	0.11
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD22	9	0.11
(1,1632)	1:58:B:VAL:HG12	2:454:F:LEU:HD23	9	0.11
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD11	9	0.11
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD12	9	0.11
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD13	9	0.11
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD21	9	0.11
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD22	9	0.11
(1,1632)	1:58:B:VAL:HG13	2:454:F:LEU:HD23	9	0.11
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD11	9	0.11
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD12	9	0.11
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD13	9	0.11
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD21	9	0.11
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD22	9	0.11
(1,1632)	1:58:B:VAL:HG21	2:454:F:LEU:HD23	9	0.11
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD11	9	0.11
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD12	9	0.11
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD13	9	0.11
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD21	9	0.11
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD22	9	0.11
(1,1632)	1:58:B:VAL:HG22	2:454:F:LEU:HD23	9	0.11
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD11	9	0.11
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD13	9	0.11
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD21	9	0.11
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD22	9	0.11
(1,1632)	1:58:B:VAL:HG23	2:454:F:LEU:HD23	9	0.11
(1,1620)	1:86:B:ILE:HD11	2:451:F:VAL:HG11	17	0.11
(1,1620)	1:86:B:ILE:HD11	2:451:F:VAL:HG12	17	0.11
(1,1620)	1:86:B:ILE:HD11	2:451:F:VAL:HG13	17	0.11
(1,1620)	1:86:B:ILE:HD11	2:451:F:VAL:HG21	17	0.11
(1,1620)	1:86:B:ILE:HD11	2:451:F:VAL:HG22	17	0.11
(1,1620)	1:86:B:ILE:HD11	2:451:F:VAL:HG23	17	0.11
(1,1620)	1:86:B:ILE:HD12	2:451:F:VAL:HG11	17	0.11
(1,1620)	1:86:B:ILE:HD12	2:451:F:VAL:HG12	17	0.11
(1,1620)	1:86:B:ILE:HD12	2:451:F:VAL:HG13	17	0.11
(1,1620)	1:86:B:ILE:HD12	2:451:F:VAL:HG21	17	0.11
(1,1620)	1:86:B:ILE:HD12	2:451:F:VAL:HG22	17	0.11
(1,1620)	1:86:B:ILE:HD12	2:451:F:VAL:HG23	17	0.11
(1,1620)	1:86:B:ILE:HD13	2:451:F:VAL:HG11	17	0.11
(1,1620)	1:86:B:ILE:HD13	2:451:F:VAL:HG12	17	0.11
(1,1620)	1:86:B:ILE:HD13	2:451:F:VAL:HG13	17	0.11
(1,1620)	1:86:B:ILE:HD13	2:451:F:VAL:HG21	17	0.11
(1,1620)	1:86:B:ILE:HD13	2:451:F:VAL:HG22	17	0.11
(1,1620)	1:86:B:ILE:HD13	2:451:F:VAL:HG23	17	0.11
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG21	17	0.11
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG22	17	0.11
(1,1618)	1:56:B:TYR:HE1	2:452:F:VAL:HG23	17	0.11
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG21	17	0.11
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG22	17	0.11
(1,1618)	1:56:B:TYR:HE2	2:452:F:VAL:HG23	17	0.11
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	2	0.11
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	2	0.11
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	2	0.11
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE1	2	0.11
(1,1610)	1:44:B:LEU:HD11	2:462:F:TYR:HE2	2	0.11
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE1	2	0.11
(1,1610)	1:44:B:LEU:HD12	2:462:F:TYR:HE2	2	0.11
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE1	2	0.11
(1,1610)	1:44:B:LEU:HD13	2:462:F:TYR:HE2	2	0.11
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD11	2	0.11
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD12	2	0.11
(1,1609)	1:74:B:PHE:HZ	2:468:F:LEU:HD13	2	0.11
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB1	1	0.11
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1604)	1:40:A:VAL:HG11	2:467:E:ALA:HB3	1	0.11
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB1	1	0.11
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB2	1	0.11
(1,1604)	1:40:A:VAL:HG12	2:467:E:ALA:HB3	1	0.11
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB1	1	0.11
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB2	1	0.11
(1,1604)	1:40:A:VAL:HG13	2:467:E:ALA:HB3	1	0.11
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB1	1	0.11
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB2	1	0.11
(1,1604)	1:40:A:VAL:HG21	2:467:E:ALA:HB3	1	0.11
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB1	1	0.11
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB2	1	0.11
(1,1604)	1:40:A:VAL:HG22	2:467:E:ALA:HB3	1	0.11
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB1	1	0.11
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB2	1	0.11
(1,1604)	1:40:A:VAL:HG23	2:467:E:ALA:HB3	1	0.11
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE1	6	0.11
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE2	6	0.11
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE3	6	0.11
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE1	6	0.11
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE2	6	0.11
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE3	6	0.11
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE1	6	0.11
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE2	6	0.11
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE3	6	0.11
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG11	15	0.11
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG12	15	0.11
(1,1595)	1:94:A:MET:HE1	2:452:E:VAL:HG13	15	0.11
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG11	15	0.11
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG12	15	0.11
(1,1595)	1:94:A:MET:HE2	2:452:E:VAL:HG13	15	0.11
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG11	15	0.11
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG12	15	0.11
(1,1595)	1:94:A:MET:HE3	2:452:E:VAL:HG13	15	0.11
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG11	19	0.11
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG12	19	0.11
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG13	19	0.11
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG21	19	0.11
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG22	19	0.11
(1,1594)	1:87:A:ALA:HB1	2:451:E:VAL:HG23	19	0.11
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG11	19	0.11
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG12	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG13	19	0.11
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG21	19	0.11
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG22	19	0.11
(1,1594)	1:87:A:ALA:HB2	2:451:E:VAL:HG23	19	0.11
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG11	19	0.11
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG12	19	0.11
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG13	19	0.11
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG21	19	0.11
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG22	19	0.11
(1,1594)	1:87:A:ALA:HB3	2:451:E:VAL:HG23	19	0.11
(1,1592)	1:89:A:ILE:HD11	2:451:E:VAL:HG11	10	0.11
(1,1592)	1:89:A:ILE:HD11	2:451:E:VAL:HG12	10	0.11
(1,1592)	1:89:A:ILE:HD11	2:451:E:VAL:HG13	10	0.11
(1,1592)	1:89:A:ILE:HD11	2:451:E:VAL:HG21	10	0.11
(1,1592)	1:89:A:ILE:HD11	2:451:E:VAL:HG22	10	0.11
(1,1592)	1:89:A:ILE:HD11	2:451:E:VAL:HG23	10	0.11
(1,1592)	1:89:A:ILE:HD12	2:451:E:VAL:HG11	10	0.11
(1,1592)	1:89:A:ILE:HD12	2:451:E:VAL:HG12	10	0.11
(1,1592)	1:89:A:ILE:HD12	2:451:E:VAL:HG13	10	0.11
(1,1592)	1:89:A:ILE:HD12	2:451:E:VAL:HG21	10	0.11
(1,1592)	1:89:A:ILE:HD12	2:451:E:VAL:HG22	10	0.11
(1,1592)	1:89:A:ILE:HD12	2:451:E:VAL:HG23	10	0.11
(1,1592)	1:89:A:ILE:HD13	2:451:E:VAL:HG11	10	0.11
(1,1592)	1:89:A:ILE:HD13	2:451:E:VAL:HG12	10	0.11
(1,1592)	1:89:A:ILE:HD13	2:451:E:VAL:HG13	10	0.11
(1,1592)	1:89:A:ILE:HD13	2:451:E:VAL:HG21	10	0.11
(1,1592)	1:89:A:ILE:HD13	2:451:E:VAL:HG22	10	0.11
(1,1592)	1:89:A:ILE:HD13	2:451:E:VAL:HG23	10	0.11
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG21	8	0.11
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG22	8	0.11
(1,1591)	1:56:A:TYR:HE1	2:452:E:VAL:HG23	8	0.11
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG21	8	0.11
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG22	8	0.11
(1,1591)	1:56:A:TYR:HE2	2:452:E:VAL:HG23	8	0.11
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	16	0.11
(1,1553)	1:133:D:PHE:H	1:136:D:LEU:H	11	0.11
(1,1537)	1:121:D:GLY:H	1:123:D:PHE:H	15	0.11
(1,1506)	1:110:D:ALA:H	1:112:D:GLU:H	7	0.11
(1,1506)	1:110:D:ALA:H	1:112:D:GLU:H	14	0.11
(1,1485)	1:97:D:CYS:H	1:100:D:ALA:H	11	0.11
(1,1458)	1:88:D:GLY:H	1:89:D:ILE:H	19	0.11
(1,1424)	1:73:D:ALA:H	1:74:D:PHE:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1414)	1:68:D:LEU:H	1:71:D:GLU:H	3	0.11
(1,1346)	1:55:D:VAL:H	1:56:D:TYR:H	16	0.11
(1,1326)	1:49:D:SER:H	1:59:D:VAL:H	18	0.11
(1,1313)	1:46:D:THR:H	1:61:D:ARG:H	3	0.11
(1,1313)	1:46:D:THR:H	1:61:D:ARG:H	7	0.11
(1,1308)	1:44:D:LEU:HD21	1:133:D:PHE:HE1	16	0.11
(1,1308)	1:44:D:LEU:HD21	1:133:D:PHE:HE2	16	0.11
(1,1308)	1:44:D:LEU:HD22	1:133:D:PHE:HE1	16	0.11
(1,1308)	1:44:D:LEU:HD22	1:133:D:PHE:HE2	16	0.11
(1,1308)	1:44:D:LEU:HD23	1:133:D:PHE:HE1	16	0.11
(1,1308)	1:44:D:LEU:HD23	1:133:D:PHE:HE2	16	0.11
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	9	0.11
(1,1275)	1:36:D:TRP:HE1	1:37:D:GLN:H	20	0.11
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	3	0.11
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	7	0.11
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	7	0.11
(1,1237)	1:23:D:PHE:HD1	1:24:D:GLU:H	18	0.11
(1,1237)	1:23:D:PHE:HD2	1:24:D:GLU:H	18	0.11
(1,1219)	1:17:D:TYR:H	1:81:D:GLY:H	7	0.11
(1,1211)	1:14:D:GLN:H	1:83:D:ILE:H	4	0.11
(1,1162)	1:126:C:LEU:H	1:127:C:ASN:H	7	0.11
(1,1129)	1:111:C:ARG:H	1:112:C:GLU:H	10	0.11
(1,1114)	1:100:C:ALA:H	1:102:C:CYS:H	14	0.11
(1,1109)	1:99:C:GLY:H	1:100:C:ALA:H	5	0.11
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	13	0.11
(1,1101)	1:97:C:CYS:H	1:98:C:LEU:H	1	0.11
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	6	0.11
(1,1033)	1:69:C:GLY:H	1:70:C:GLU:H	14	0.11
(1,1029)	1:68:C:LEU:H	1:71:C:GLU:H	2	0.11
(1,1028)	1:68:C:LEU:H	1:70:C:GLU:H	3	0.11
(1,1013)	1:66:C:ALA:H	1:73:C:ALA:H	2	0.11
(1,985)	1:60:C:LEU:H	1:81:C:GLY:H	7	0.11
(1,985)	1:60:C:LEU:H	1:81:C:GLY:H	11	0.11
(1,972)	1:58:C:VAL:H	1:59:C:VAL:H	13	0.11
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	18	0.11
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	18	0.11
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	18	0.11
(1,899)	1:41:C:LYS:H	1:67:C:SER:H	9	0.11
(1,885)	1:36:C:TRP:H	1:37:C:GLN:H	18	0.11
(1,878)	1:32:C:PHE:H	1:34:C:LYS:H	20	0.11
(1,845)	1:23:C:PHE:H	1:24:C:GLU:H	2	0.11
(1,844)	1:22:C:SER:H	1:23:D:PHE:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:21:C:ILE:H	1:23:D:PHE:H	12	0.11
(1,805)	1:11:C:PHE:HE1	1:102:C:CYS:H	19	0.11
(1,805)	1:11:C:PHE:HE2	1:102:C:CYS:H	19	0.11
(1,767)	1:134:B:ASP:H	1:136:B:LEU:H	10	0.11
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	2	0.11
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	6	0.11
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	8	0.11
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	10	0.11
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	10	0.11
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	10	0.11
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	10	0.11
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	10	0.11
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	10	0.11
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	10	0.11
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	10	0.11
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	10	0.11
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	5	0.11
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	7	0.11
(1,750)	1:121:B:GLY:H	1:123:B:PHE:H	20	0.11
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	11	0.11
(1,719)	1:110:B:ALA:H	1:111:B:ARG:H	16	0.11
(1,709)	1:100:B:ALA:H	1:102:B:CYS:H	8	0.11
(1,706)	1:99:B:GLY:H	1:101:B:TYR:H	15	0.11
(1,697)	1:97:B:CYS:H	1:99:B:GLY:H	11	0.11
(1,684)	1:94:B:MET:H	1:96:B:HIS:H	10	0.11
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE1	9	0.11
(1,662)	1:83:B:ILE:H	1:84:B:PHE:HE2	9	0.11
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD21	8	0.11
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD22	8	0.11
(1,639)	1:74:B:PHE:H	1:75:B:LEU:HD23	8	0.11
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	7	0.11
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	10	0.11
(1,549)	1:55:B:VAL:H	1:56:B:TYR:H	17	0.11
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	1	0.11
(1,530)	1:49:B:SER:H	1:57:B:GLU:H	19	0.11
(1,522)	1:47:B:ALA:H	1:48:B:SER:H	4	0.11
(1,502)	1:42:B:LEU:HD21	1:43:B:ASP:H	19	0.11
(1,502)	1:42:B:LEU:HD22	1:43:B:ASP:H	19	0.11
(1,502)	1:42:B:LEU:HD23	1:43:B:ASP:H	19	0.11
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	14	0.11
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	14	0.11
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	14	0.11
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	14	0.11
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	14	0.11
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	14	0.11
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	14	0.11
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	14	0.11
(1,405)	1:11:B:PHE:HD1	1:12:B:GLN:H	3	0.11
(1,405)	1:11:B:PHE:HD2	1:12:B:GLN:H	3	0.11
(1,395)	1:140:A:TYR:H	1:141:A:LEU:H	11	0.11
(1,361)	1:126:A:LEU:H	1:127:A:ASN:H	17	0.11
(1,359)	1:122:A:THR:H	1:18:B:THR:H	7	0.11
(1,356)	1:121:A:GLY:H	1:123:A:PHE:H	4	0.11
(1,356)	1:121:A:GLY:H	1:123:A:PHE:H	14	0.11
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	13	0.11
(1,315)	1:101:A:TYR:H	1:102:A:CYS:H	2	0.11
(1,308)	1:99:A:GLY:H	1:101:A:TYR:H	10	0.11
(1,308)	1:99:A:GLY:H	1:101:A:TYR:H	13	0.11
(1,304)	1:98:A:LEU:H	1:102:A:CYS:H	11	0.11
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	14	0.11
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	17	0.11
(1,293)	1:96:A:HIS:H	1:97:A:CYS:H	6	0.11
(1,266)	1:85:A:SER:H	1:86:A:ILE:H	2	0.11
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	19	0.11
(1,226)	1:68:A:LEU:H	1:73:A:ALA:H	7	0.11
(1,222)	1:68:A:LEU:H	1:69:A:GLY:H	16	0.11
(1,222)	1:68:A:LEU:H	1:69:A:GLY:H	18	0.11
(1,213)	1:66:A:ALA:H	1:76:A:CYS:H	14	0.11
(1,212)	1:66:A:ALA:H	1:74:A:PHE:HE1	10	0.11
(1,212)	1:66:A:ALA:H	1:74:A:PHE:HE2	10	0.11
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	17	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB1	13	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB2	13	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB3	13	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB1	13	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB2	13	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB3	13	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB1	13	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB2	13	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB3	13	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB1	20	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB2	20	0.11
(1,196)	1:62:A:VAL:HG21	1:110:A:ALA:HB3	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB1	20	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB2	20	0.11
(1,196)	1:62:A:VAL:HG22	1:110:A:ALA:HB3	20	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB1	20	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB2	20	0.11
(1,196)	1:62:A:VAL:HG23	1:110:A:ALA:HB3	20	0.11
(1,183)	1:60:A:LEU:H	1:82:A:GLY:H	17	0.11
(1,141)	1:51:A:LEU:H	1:55:A:VAL:H	9	0.11
(1,139)	1:50:A:GLN:H	1:57:A:GLU:H	6	0.11
(1,139)	1:50:A:GLN:H	1:57:A:GLU:H	7	0.11
(1,125)	1:45:A:ASP:H	1:46:A:THR:H	20	0.11
(1,122)	1:44:A:LEU:HD21	1:45:A:ASP:H	15	0.11
(1,122)	1:44:A:LEU:HD22	1:45:A:ASP:H	15	0.11
(1,122)	1:44:A:LEU:HD23	1:45:A:ASP:H	15	0.11
(1,95)	1:39:A:GLU:H	1:40:A:VAL:H	18	0.11
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD21	18	0.11
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD22	18	0.11
(1,94)	1:37:A:GLN:H	1:68:A:LEU:HD23	18	0.11
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	5	0.11
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	12	0.11
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	7	0.1
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	7	0.1
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	7	0.1
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	7	0.1
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	7	0.1
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	7	0.1
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE1	14	0.1
(1,1679)	1:136:D:LEU:HD21	2:461:H:PHE:HE2	14	0.1
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE1	14	0.1
(1,1679)	1:136:D:LEU:HD22	2:461:H:PHE:HE2	14	0.1
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE1	14	0.1
(1,1679)	1:136:D:LEU:HD23	2:461:H:PHE:HE2	14	0.1
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG11	11	0.1
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG12	11	0.1
(1,1676)	1:94:D:MET:HE1	2:452:H:VAL:HG13	11	0.1
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG11	11	0.1
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG12	11	0.1
(1,1676)	1:94:D:MET:HE2	2:452:H:VAL:HG13	11	0.1
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG11	11	0.1
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG12	11	0.1
(1,1676)	1:94:D:MET:HE3	2:452:H:VAL:HG13	11	0.1
(1,1670)	1:98:D:LEU:HD11	2:454:H:LEU:HD21	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1670)	1:98:D:LEU:HD11	2:454:H:LEU:HD22	15	0.1
(1,1670)	1:98:D:LEU:HD11	2:454:H:LEU:HD23	15	0.1
(1,1670)	1:98:D:LEU:HD12	2:454:H:LEU:HD21	15	0.1
(1,1670)	1:98:D:LEU:HD12	2:454:H:LEU:HD22	15	0.1
(1,1670)	1:98:D:LEU:HD12	2:454:H:LEU:HD23	15	0.1
(1,1670)	1:98:D:LEU:HD13	2:454:H:LEU:HD21	15	0.1
(1,1670)	1:98:D:LEU:HD13	2:454:H:LEU:HD22	15	0.1
(1,1670)	1:98:D:LEU:HD13	2:454:H:LEU:HD23	15	0.1
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	8	0.1
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	8	0.1
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	8	0.1
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD11	19	0.1
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD12	19	0.1
(1,1666)	1:36:D:TRP:HZ2	2:470:H:LEU:HD13	19	0.1
(1,1664)	1:44:D:LEU:HD11	2:462:H:TYR:HE1	14	0.1
(1,1664)	1:44:D:LEU:HD11	2:462:H:TYR:HE2	14	0.1
(1,1664)	1:44:D:LEU:HD12	2:462:H:TYR:HE1	14	0.1
(1,1664)	1:44:D:LEU:HD12	2:462:H:TYR:HE2	14	0.1
(1,1664)	1:44:D:LEU:HD13	2:462:H:TYR:HE1	14	0.1
(1,1664)	1:44:D:LEU:HD13	2:462:H:TYR:HE2	14	0.1
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE1	10	0.1
(1,1652)	1:136:C:LEU:HD21	2:461:G:PHE:HE2	10	0.1
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE1	10	0.1
(1,1652)	1:136:C:LEU:HD22	2:461:G:PHE:HE2	10	0.1
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE1	10	0.1
(1,1652)	1:136:C:LEU:HD23	2:461:G:PHE:HE2	10	0.1
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD11	1	0.1
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD12	1	0.1
(1,1651)	1:133:C:PHE:HD1	2:460:G:LEU:HD13	1	0.1
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD11	1	0.1
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD12	1	0.1
(1,1651)	1:133:C:PHE:HD2	2:460:G:LEU:HD13	1	0.1
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG11	16	0.1
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG12	16	0.1
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG13	16	0.1
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG11	16	0.1
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG12	16	0.1
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG13	16	0.1
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG11	16	0.1
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG12	16	0.1
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG13	16	0.1
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG11	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG12	17	0.1
(1,1649)	1:94:C:MET:HE1	2:452:G:VAL:HG13	17	0.1
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG11	17	0.1
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG12	17	0.1
(1,1649)	1:94:C:MET:HE2	2:452:G:VAL:HG13	17	0.1
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG11	17	0.1
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG12	17	0.1
(1,1649)	1:94:C:MET:HE3	2:452:G:VAL:HG13	17	0.1
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE1	11	0.1
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE2	11	0.1
(1,1630)	1:128:B:LEU:HD11	2:464:F:MET:HE3	11	0.1
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE1	11	0.1
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE2	11	0.1
(1,1630)	1:128:B:LEU:HD12	2:464:F:MET:HE3	11	0.1
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE1	11	0.1
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE2	11	0.1
(1,1630)	1:128:B:LEU:HD13	2:464:F:MET:HE3	11	0.1
(1,1628)	1:131:B:VAL:HG21	2:462:F:TYR:HD1	20	0.1
(1,1628)	1:131:B:VAL:HG21	2:462:F:TYR:HD2	20	0.1
(1,1628)	1:131:B:VAL:HG22	2:462:F:TYR:HD1	20	0.1
(1,1628)	1:131:B:VAL:HG22	2:462:F:TYR:HD2	20	0.1
(1,1628)	1:131:B:VAL:HG23	2:462:F:TYR:HD1	20	0.1
(1,1628)	1:131:B:VAL:HG23	2:462:F:TYR:HD2	20	0.1
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	13	0.1
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	13	0.1
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	13	0.1
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	13	0.1
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	13	0.1
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	13	0.1
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE1	20	0.1
(1,1625)	1:136:B:LEU:HD21	2:461:F:PHE:HE2	20	0.1
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE1	20	0.1
(1,1625)	1:136:B:LEU:HD22	2:461:F:PHE:HE2	20	0.1
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE1	20	0.1
(1,1625)	1:136:B:LEU:HD23	2:461:F:PHE:HE2	20	0.1
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD11	1	0.1
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD12	1	0.1
(1,1612)	1:36:B:TRP:HZ2	2:470:F:LEU:HD13	1	0.1
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD11	10	0.1
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD12	10	0.1
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD13	10	0.1
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD21	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD22	10	0.1
(1,1608)	1:98:A:LEU:HD11	2:454:E:LEU:HD23	10	0.1
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD11	10	0.1
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD12	10	0.1
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD13	10	0.1
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD21	10	0.1
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD22	10	0.1
(1,1608)	1:98:A:LEU:HD12	2:454:E:LEU:HD23	10	0.1
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD11	10	0.1
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD12	10	0.1
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD13	10	0.1
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD21	10	0.1
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD22	10	0.1
(1,1608)	1:98:A:LEU:HD13	2:454:E:LEU:HD23	10	0.1
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD11	10	0.1
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD12	10	0.1
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD13	10	0.1
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD21	10	0.1
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD22	10	0.1
(1,1608)	1:98:A:LEU:HD21	2:454:E:LEU:HD23	10	0.1
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD11	10	0.1
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD12	10	0.1
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD13	10	0.1
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD21	10	0.1
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD22	10	0.1
(1,1608)	1:98:A:LEU:HD22	2:454:E:LEU:HD23	10	0.1
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD11	10	0.1
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD12	10	0.1
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD13	10	0.1
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD21	10	0.1
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD22	10	0.1
(1,1608)	1:98:A:LEU:HD23	2:454:E:LEU:HD23	10	0.1
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE1	10	0.1
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE2	10	0.1
(1,1603)	1:128:A:LEU:HD11	2:464:E:MET:HE3	10	0.1
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE1	10	0.1
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE2	10	0.1
(1,1603)	1:128:A:LEU:HD12	2:464:E:MET:HE3	10	0.1
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE1	10	0.1
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE2	10	0.1
(1,1603)	1:128:A:LEU:HD13	2:464:E:MET:HE3	10	0.1
(1,1558)	1:134:D:ASP:H	1:136:D:LEU:H	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE1	15	0.1
(1,1548)	1:131:D:VAL:H	1:133:D:PHE:HE2	15	0.1
(1,1505)	1:110:D:ALA:H	1:111:D:ARG:H	20	0.1
(1,1480)	1:96:D:HIS:H	1:98:D:LEU:H	8	0.1
(1,1271)	1:35:D:ASP:H	1:36:D:TRP:H	11	0.1
(1,1248)	1:28:D:ALA:H	1:31:D:VAL:H	1	0.1
(1,1106)	1:98:C:LEU:H	1:100:C:ALA:H	16	0.1
(1,1104)	1:97:C:CYS:H	1:101:C:TYR:H	20	0.1
(1,1073)	1:87:C:ALA:H	1:88:C:GLY:H	14	0.1
(1,1035)	1:70:C:GLU:H	1:71:C:GLU:H	8	0.1
(1,993)	1:61:C:ARG:H	1:62:C:VAL:H	4	0.1
(1,965)	1:56:C:TYR:H	1:84:C:PHE:H	3	0.1
(1,960)	1:55:C:VAL:H	1:56:C:TYR:H	6	0.1
(1,944)	1:51:C:LEU:H	1:56:C:TYR:H	10	0.1
(1,914)	1:44:C:LEU:HD11	1:133:C:PHE:HE1	10	0.1
(1,914)	1:44:C:LEU:HD11	1:133:C:PHE:HE2	10	0.1
(1,914)	1:44:C:LEU:HD12	1:133:C:PHE:HE1	10	0.1
(1,914)	1:44:C:LEU:HD12	1:133:C:PHE:HE2	10	0.1
(1,914)	1:44:C:LEU:HD13	1:133:C:PHE:HE1	10	0.1
(1,914)	1:44:C:LEU:HD13	1:133:C:PHE:HE2	10	0.1
(1,904)	1:42:C:LEU:HD21	1:43:C:ASP:H	9	0.1
(1,904)	1:42:C:LEU:HD22	1:43:C:ASP:H	9	0.1
(1,904)	1:42:C:LEU:HD23	1:43:C:ASP:H	9	0.1
(1,885)	1:36:C:TRP:H	1:37:C:GLN:H	8	0.1
(1,866)	1:30:C:HIS:H	1:32:C:PHE:H	17	0.1
(1,790)	1:9:C:MET:H	1:10:C:THR:H	20	0.1
(1,766)	1:134:B:ASP:H	1:135:B:ALA:H	18	0.1
(1,757)	1:127:B:ASN:H	1:128:B:LEU:H	9	0.1
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD21	7	0.1
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD22	7	0.1
(1,756)	1:126:B:LEU:HD21	1:128:B:LEU:HD23	7	0.1
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD21	7	0.1
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD22	7	0.1
(1,756)	1:126:B:LEU:HD22	1:128:B:LEU:HD23	7	0.1
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD21	7	0.1
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD22	7	0.1
(1,756)	1:126:B:LEU:HD23	1:128:B:LEU:HD23	7	0.1
(1,720)	1:110:B:ALA:H	1:112:B:GLU:H	17	0.1
(1,682)	1:93:B:GLN:H	1:96:B:HIS:H	10	0.1
(1,679)	1:92:B:THR:H	1:94:B:MET:H	4	0.1
(1,630)	1:69:B:GLY:H	1:71:B:GLU:H	9	0.1
(1,608)	1:66:B:ALA:H	1:74:B:PHE:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:64:B:VAL:H	1:65:B:THR:H	14	0.1
(1,535)	1:51:B:LEU:H	1:52:B:ALA:H	16	0.1
(1,531)	1:49:B:SER:H	1:58:B:VAL:H	10	0.1
(1,522)	1:47:B:ALA:H	1:48:B:SER:H	13	0.1
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD11	4	0.1
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD12	4	0.1
(1,461)	1:31:B:VAL:HG21	1:68:B:LEU:HD13	4	0.1
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD11	4	0.1
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD12	4	0.1
(1,461)	1:31:B:VAL:HG22	1:68:B:LEU:HD13	4	0.1
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD11	4	0.1
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD12	4	0.1
(1,461)	1:31:B:VAL:HG23	1:68:B:LEU:HD13	4	0.1
(1,410)	1:12:B:GLN:H	1:13:B:ILE:H	15	0.1
(1,406)	1:11:B:PHE:HE1	1:12:B:GLN:H	4	0.1
(1,406)	1:11:B:PHE:HE2	1:12:B:GLN:H	4	0.1
(1,354)	1:119:A:SER:H	1:123:A:PHE:H	16	0.1
(1,320)	1:110:A:ALA:H	1:111:A:ARG:H	9	0.1
(1,303)	1:98:A:LEU:H	1:101:A:TYR:H	1	0.1
(1,301)	1:98:A:LEU:H	1:99:A:GLY:H	18	0.1
(1,297)	1:97:A:CYS:H	1:98:A:LEU:H	12	0.1
(1,295)	1:96:A:HIS:H	1:99:A:GLY:H	18	0.1
(1,289)	1:95:A:ALA:H	1:98:A:LEU:H	16	0.1
(1,278)	1:92:A:THR:H	1:93:A:GLN:H	13	0.1
(1,231)	1:69:A:GLY:H	1:70:A:GLU:H	9	0.1
(1,226)	1:68:A:LEU:H	1:73:A:ALA:H	17	0.1
(1,199)	1:64:A:VAL:H	1:65:A:THR:H	13	0.1
(1,86)	1:36:A:TRP:H	1:37:A:GLN:H	15	0.1
(1,66)	1:28:A:ALA:H	1:30:A:HIS:H	12	0.1
(1,43)	1:21:A:ILE:H	1:22:A:SER:H	18	0.1
(1,36)	1:18:A:THR:H	1:122:B:THR:H	8	0.1
(1,23)	1:15:A:ARG:H	1:83:A:ILE:H	13	0.1
(1,18)	1:14:A:GLN:H	1:83:A:ILE:H	10	0.1

10 Dihedral-angle violation analysis

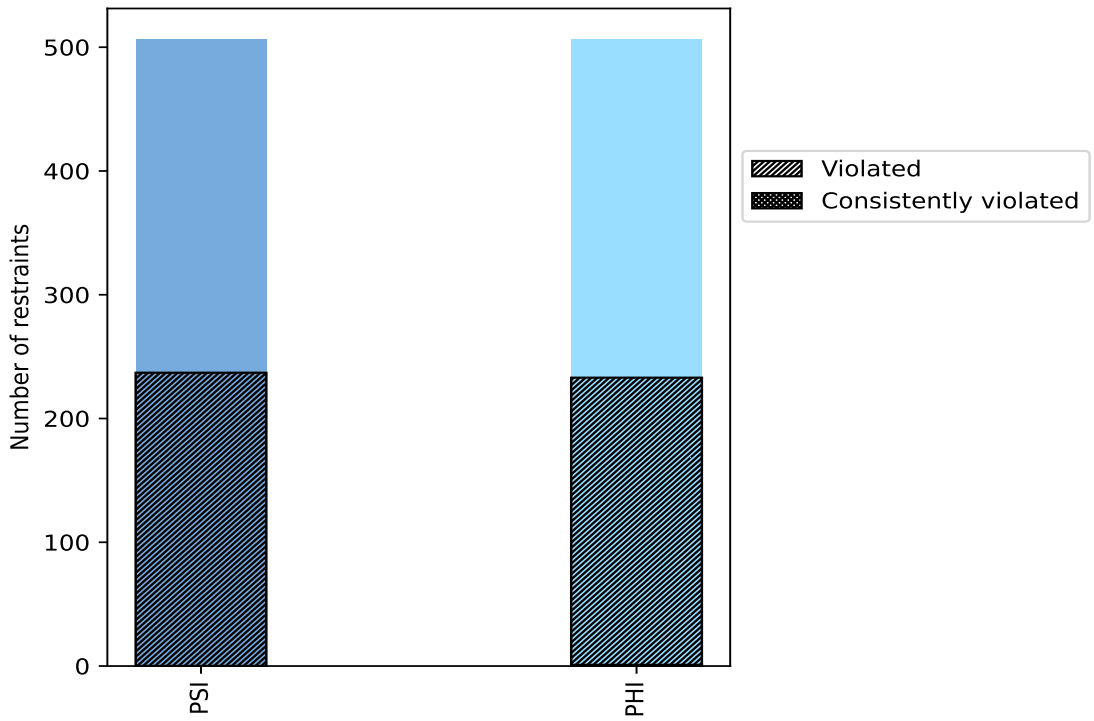
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	506	50.0	237	46.8	23.4	0	0.0	0.0
PHI	506	50.0	233	46.0	23.0	1	0.2	0.1
Total	1012	100.0	470	46.4	46.4	1	0.1	0.1

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



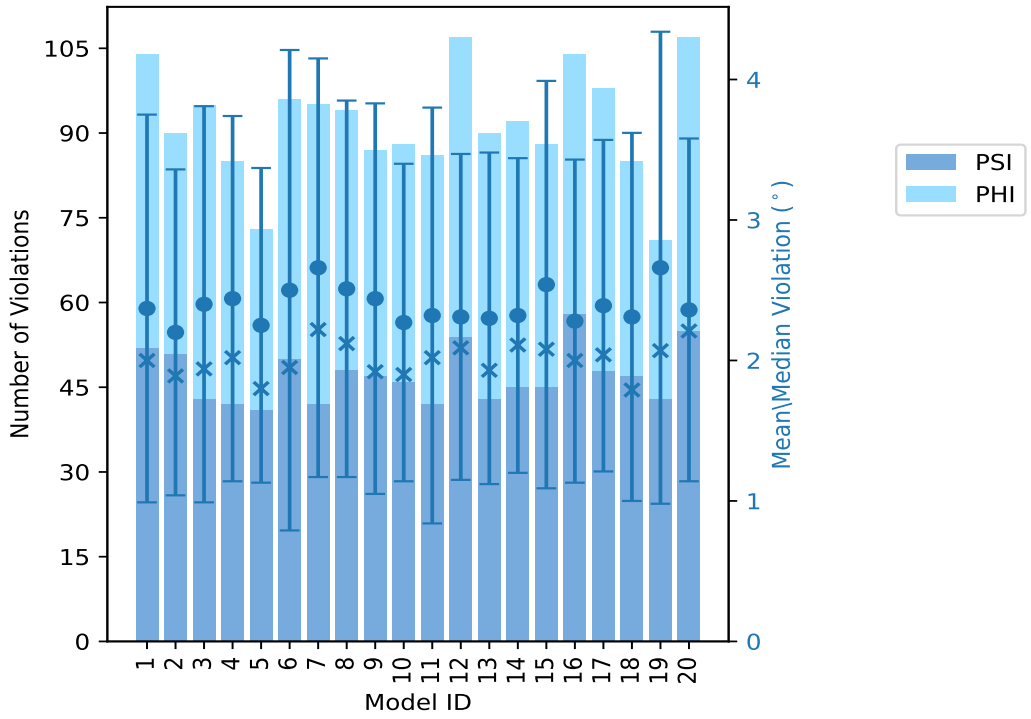
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	52	52	104	2.37	9.43	1.38	2.0
2	51	39	90	2.2	8.21	1.16	1.89
3	43	52	95	2.4	8.71	1.41	1.94
4	42	43	85	2.44	7.65	1.3	2.02
5	41	32	73	2.25	5.42	1.12	1.8
6	50	46	96	2.5	12.15	1.71	1.95
7	42	53	95	2.66	8.13	1.49	2.22
8	48	46	94	2.51	7.95	1.34	2.12
9	47	40	87	2.44	8.63	1.39	1.92
10	46	42	88	2.27	6.7	1.13	1.9
11	42	44	86	2.32	11.46	1.48	2.02
12	54	53	107	2.31	7.26	1.16	2.09
13	43	47	90	2.3	7.47	1.18	1.93
14	45	47	92	2.32	5.92	1.12	2.11
15	45	43	88	2.54	8.59	1.45	2.08
16	58	46	104	2.28	6.95	1.15	2.0
17	48	50	98	2.39	7.9	1.18	2.04
18	47	38	85	2.31	9.31	1.31	1.79
19	43	28	71	2.66	11.46	1.68	2.07
20	55	52	107	2.36	8.26	1.22	2.21

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[1]	%
70	82	152	1	5.0
31	32	63	2	10.0
38	24	62	3	15.0
22	25	47	4	20.0
17	13	30	5	25.0
13	20	33	6	30.0
10	10	20	7	35.0
10	4	14	8	40.0
7	6	13	9	45.0
4	3	7	10	50.0
6	3	9	11	55.0

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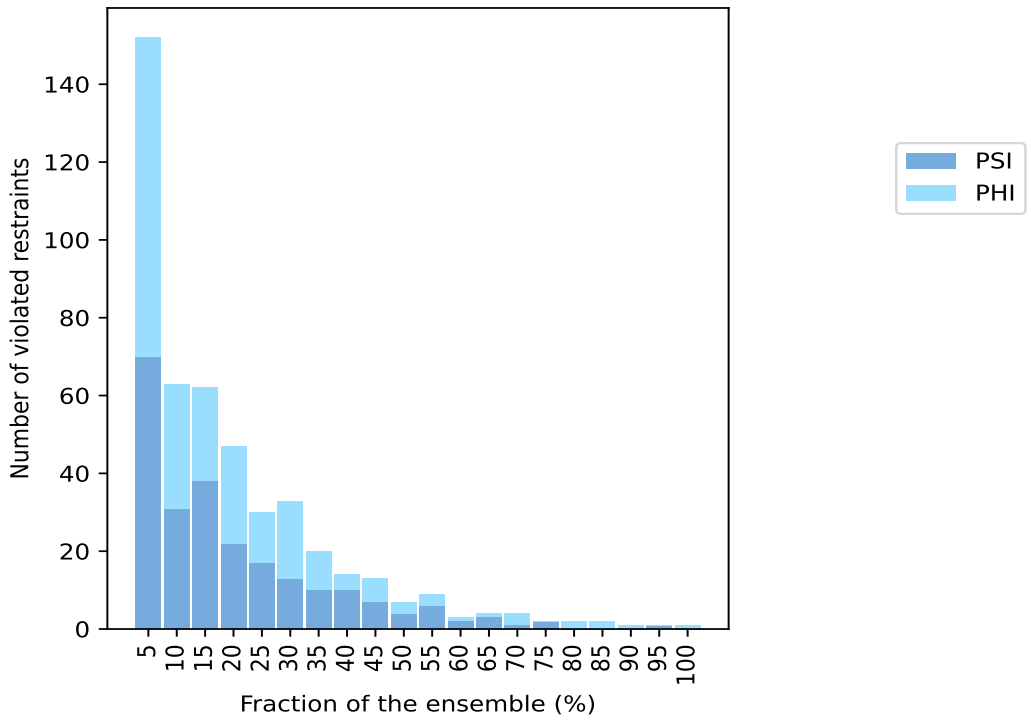
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
2	1	3	12	60.0
3	1	4	13	65.0
1	3	4	14	70.0
2	0	2	15	75.0
0	2	2	16	80.0
0	2	2	17	85.0
0	1	1	18	90.0
1	0	1	19	95.0
0	1	1	20	100.0

[1] Number of models with violations

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

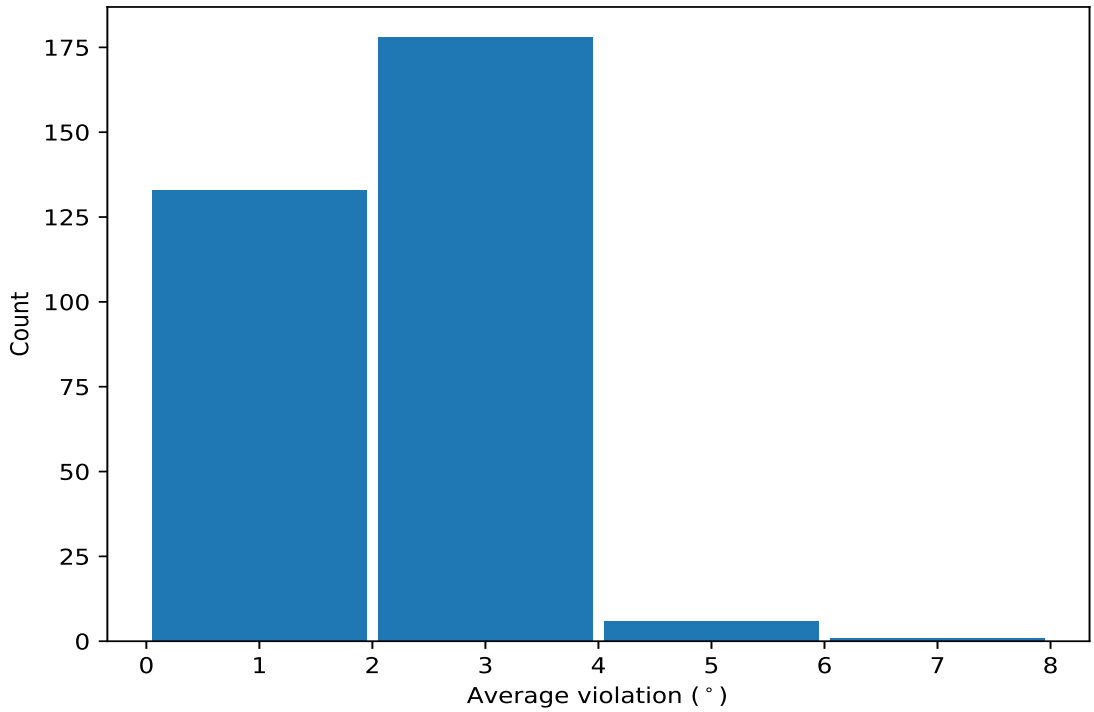


10.4 Most violated dihedral-angle restraints in the ensemble

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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	20	7.03	2.62	7.6
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	19	5.14	2.31	4.33
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	18	2.12	0.71	2.14
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	17	3.72	1.22	3.3
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	17	3.66	1.19	3.92
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	16	3.64	1.1	3.67
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	16	2.97	1.16	2.7
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	15	3.76	1.35	3.87
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	15	3.09	1.72	2.84
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	14	3.04	1.49	2.6
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	14	2.73	0.87	2.45
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	14	2.54	1.02	2.26
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	14	2.12	0.69	2.04
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	13	4.01	1.7	4.52
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	13	3.09	1.27	3.17
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	13	2.91	0.91	2.8
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	13	2.56	1.42	2.13
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	12	2.76	0.95	3.16
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	12	2.73	1.4	2.32
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	12	2.72	1.25	2.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	11	4.02	1.17	4.46
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	11	3.65	2.22	3.5
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	11	3.45	1.87	3.04
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	11	2.58	1.31	2.14
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	11	2.13	0.82	1.93
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	11	1.98	0.53	1.96
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	11	1.96	0.65	2.03
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	11	1.82	0.59	1.67
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	11	1.8	0.59	1.65
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	10	3.15	1.84	2.72
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	10	2.83	0.97	3.06
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	10	2.61	0.97	2.48
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	10	2.5	1.39	1.78
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	10	2.2	0.93	2.13
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	10	1.87	0.69	1.8
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	10	1.65	0.57	1.46
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	9	3.41	1.84	3.23
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	9	2.94	1.17	2.75
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	9	2.7	0.85	2.53
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	9	2.58	0.78	2.49
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	9	2.56	0.68	2.49
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	9	2.56	1.52	2.56
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	9	2.53	1.19	2.17
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	9	2.26	0.9	2.01
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	9	2.14	0.76	2.02
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	9	1.96	0.46	1.99
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	9	1.92	0.45	2.0
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	9	1.8	0.7	1.63
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	9	1.59	0.9	1.16
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	8	3.3	1.73	2.86
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	8	2.92	1.07	2.97
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	8	2.78	0.94	2.82
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	8	2.6	0.83	2.65
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	8	2.55	1.05	2.09
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	8	2.49	1.27	2.1
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	8	2.46	0.97	2.54
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	8	2.39	0.92	2.61
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	8	2.37	0.71	2.31
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	8	2.17	1.34	1.77
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	8	2.07	0.67	1.8
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	8	1.78	0.42	1.64
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	8	1.74	0.5	1.6
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	8	1.65	0.49	1.42
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	7	3.86	1.28	3.55
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	7	3.3	0.7	3.26
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	7	2.63	1.47	1.96
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	7	2.42	1.14	2.28
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	7	2.4	1.1	1.94
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	7	2.38	0.67	2.17
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	7	2.3	0.71	2.31
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	7	2.3	1.67	1.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	7	2.23	0.88	2.19
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	7	2.22	0.66	2.21
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	7	2.09	0.69	1.84
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	7	2.08	1.11	1.47
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	7	2.07	0.84	1.95
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	7	2.02	1.0	1.68
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	7	2.01	0.69	1.98
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	7	1.96	1.01	1.74
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	7	1.82	0.37	1.81
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	7	1.8	0.72	1.71
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	7	1.71	0.54	1.44
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	7	1.66	0.58	1.45
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	6	4.04	2.22	3.92
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	6	3.09	0.93	2.96
(1,321)	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1:46:B:THR:N	6	2.93	1.18	2.91
(1,104)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	6	2.67	0.74	2.2
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	6	2.61	0.77	2.59
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	6	2.57	1.54	2.19
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	6	2.54	1.07	1.94
(1,645)	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	1:82:C:GLY:N	6	2.37	0.53	2.34
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	6	2.37	0.69	2.18
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	6	2.34	1.06	2.06
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	6	2.32	0.82	2.27
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	6	2.31	0.79	2.42
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	6	2.25	0.79	2.14
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	6	2.19	0.78	2.04
(1,70)	1:46:A:THR:C	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	6	2.16	0.77	2.42
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	6	2.08	0.9	1.78
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	6	2.07	0.79	2.0
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	6	2.04	0.64	1.99
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	6	2.04	0.52	1.88
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	6	2.02	1.03	1.5
(1,37)	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1:29:A:PRO:N	6	1.88	1.01	1.56
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	6	1.85	0.36	1.84
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	6	1.84	0.77	1.52
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	6	1.81	0.53	1.64
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	6	1.8	0.54	1.72
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	6	1.79	0.68	1.69
(1,880)	1:73:D:ALA:C	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	6	1.72	0.49	1.62
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	6	1.63	0.44	1.57
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	6	1.59	0.11	1.61
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	6	1.57	0.4	1.48
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	6	1.5	0.47	1.37
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	6	1.47	0.41	1.44
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	6	1.32	0.3	1.17
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	5	4.2	2.09	3.99
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	5	3.12	1.76	2.9
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	5	2.99	1.37	2.92
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	5	2.75	0.78	2.49
(1,252)	1:141:A:LEU:C	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	5	2.68	1.48	2.37
(1,17)	1:17:A:TYR:N	1:17:A:TYR:CA	1:17:A:TYR:C	1:18:A:THR:N	5	2.6	1.04	2.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	5	2.47	0.79	2.35
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	5	2.43	0.57	2.25
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	5	2.31	0.8	2.1
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	5	2.29	0.83	2.04
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	5	2.27	0.58	2.7
(1,324)	1:46:B:THR:C	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	5	2.17	0.56	2.0
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	5	2.11	0.34	2.2
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	5	2.1	0.63	1.9
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	5	2.02	1.04	1.52
(1,109)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:SER:N	5	1.97	0.58	1.9
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	5	1.94	0.77	1.76
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	5	1.9	0.39	1.95
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	5	1.85	0.65	1.57
(1,901)	1:84:D:PHE:N	1:84:D:PHE:CA	1:84:D:PHE:C	1:85:D:SER:N	5	1.84	0.39	1.9
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	5	1.82	0.76	1.56
(1,655)	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	1:87:C:ALA:N	5	1.8	0.47	1.59
(1,95)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:LEU:N	5	1.72	0.67	1.32
(1,579)	1:48:C:SER:N	1:48:C:SER:CA	1:48:C:SER:C	1:49:C:SER:N	5	1.72	0.67	1.59
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	5	1.62	0.51	1.47
(1,96)	1:59:A:VAL:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	5	1.61	0.52	1.45
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	5	1.48	0.25	1.33
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	5	1.48	0.36	1.64
(1,305)	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1:37:B:GLN:N	5	1.41	0.38	1.33
(1,855)	1:61:D:ARG:N	1:61:D:ARG:CA	1:61:D:ARG:C	1:62:D:VAL:N	5	1.17	0.14	1.1
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	4	3.92	2.51	3.6
(1,407)	1:88:B:GLY:N	1:88:B:GLY:CA	1:88:B:GLY:C	1:89:B:ILE:N	4	3.51	1.78	3.5
(1,415)	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	1:93:B:GLN:N	4	3.36	1.95	2.56
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	4	3.14	2.22	2.09
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	4	2.84	2.23	1.78
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	4	2.8	1.69	2.13
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	4	2.68	0.48	2.58
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	4	2.63	0.58	2.67
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	4	2.62	0.97	2.33
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	4	2.57	0.7	2.82
(1,523)	1:17:C:TYR:N	1:17:C:TYR:CA	1:17:C:TYR:C	1:18:C:THR:N	4	2.52	0.89	2.34
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	4	2.43	0.41	2.26
(1,741)	1:133:C:PHE:N	1:133:C:PHE:CA	1:133:C:PHE:C	1:134:C:ASP:N	4	2.36	1.49	1.64
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	4	2.32	0.59	2.36
(1,362)	1:65:B:THR:C	1:66:B:ALA:N	1:66:B:ALA:CA	1:66:B:ALA:C	4	2.28	0.67	2.07
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	4	2.28	0.33	2.37
(1,108)	1:65:A:THR:C	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	4	2.27	0.93	2.0
(1,101)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:THR:N	4	2.26	0.3	2.24
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	4	2.24	1.21	1.78
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	4	2.24	0.5	2.44
(1,819)	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	1:44:D:LEU:N	4	2.15	0.33	2.19
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	4	2.13	0.94	1.9
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	4	2.12	0.47	2.04
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	4	2.06	0.17	2.03
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	4	2.05	0.62	2.18
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	4	2.04	0.7	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	2.03	0.55	2.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,644)	1:80:C:GLN:C	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	4	2.02	0.2	2.06
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	4	2.01	0.59	1.9
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	4	1.98	0.22	1.94
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	4	1.98	0.39	1.77
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	4	1.96	0.3	1.9
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	4	1.88	0.61	1.76
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	4	1.87	0.19	1.98
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	4	1.84	0.6	1.57
(1,761)	1:11:D:PHE:N	1:11:D:PHE:CA	1:11:D:PHE:C	1:12:D:GLN:N	4	1.81	0.75	1.75
(1,559)	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	1:38:C:PRO:N	4	1.71	0.43	1.72
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	4	1.7	0.36	1.58
(1,92)	1:57:A:GLU:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	4	1.69	0.1	1.71
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	4	1.68	0.27	1.58
(1,974)	1:122:D:THR:C	1:123:D:PHE:N	1:123:D:PHE:CA	1:123:D:PHE:C	4	1.63	0.36	1.69
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	4	1.58	0.38	1.55
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	4	1.56	0.06	1.54
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	4	1.51	0.48	1.33
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	4	1.4	0.29	1.44
(1,102)	1:62:A:VAL:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	4	1.4	0.37	1.27
(1,810)	1:38:D:PRO:C	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	4	1.26	0.24	1.23
(1,728)	1:125:C:GLN:C	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	3	3.97	1.06	4.52
(1,130)	1:76:A:CYS:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	3	3.3	1.44	3.55
(1,538)	1:24:C:GLU:C	1:25:C:ALA:N	1:25:C:ALA:CA	1:25:C:ALA:C	3	3.23	1.57	2.96
(1,38)	1:29:A:PRO:C	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	3	3.06	1.77	1.88
(1,224)	1:126:A:LEU:C	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	3	3.04	1.04	2.34
(1,815)	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	1:42:D:LEU:N	3	2.91	1.25	3.12
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	3	2.84	1.55	2.63
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	3	2.8	1.08	2.2
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	3	2.65	1.52	2.04
(1,887)	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	1:78:D:VAL:N	3	2.64	1.34	1.8
(1,311)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:LYS:N	3	2.63	0.92	2.91
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	3	2.56	1.77	1.45
(1,372)	1:70:B:GLU:C	1:71:B:GLU:N	1:71:B:GLU:CA	1:71:B:GLU:C	3	2.44	0.74	2.45
(1,570)	1:43:C:ASP:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	3	2.43	0.96	1.97
(1,660)	1:88:C:GLY:C	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	3	2.38	0.57	2.39
(1,22)	1:19:A:LYS:C	1:20:A:ASP:N	1:20:A:ASP:CA	1:20:A:ASP:C	3	2.37	0.45	2.16
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	3	2.34	1.28	1.57
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	3	2.31	1.21	1.97
(1,119)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:THR:N	3	2.28	0.33	2.3
(1,983)	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	1:129:D:ALA:N	3	2.24	0.35	2.21
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	3	2.21	1.26	1.53
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	3	2.15	1.36	1.32
(1,163)	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	1:94:A:MET:N	3	2.04	0.93	1.72
(1,610)	1:63:C:THR:C	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	3	2.04	0.28	2.09
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	3	2.02	0.22	2.05
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	3	2.02	0.15	2.01
(1,383)	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	1:77:B:GLU:N	3	2.0	0.87	1.56
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	3	1.98	0.1	1.92
(1,769)	1:15:D:ARG:N	1:15:D:ARG:CA	1:15:D:ARG:C	1:16:D:ILE:N	3	1.96	0.71	2.17
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	3	1.95	0.56	2.33
(1,489)	1:133:B:PHE:N	1:133:B:PHE:CA	1:133:B:PHE:C	1:134:B:ASP:N	3	1.92	0.28	2.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	3	1.91	0.59	1.55
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	3	1.89	0.72	1.6
(1,476)	1:125:B:GLN:C	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	3	1.85	0.79	1.32
(1,403)	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1:87:B:ALA:N	3	1.85	0.53	2.11
(1,511)	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	1:12:C:GLN:N	3	1.83	0.75	1.66
(1,315)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:ASP:N	3	1.81	0.28	1.93
(1,905)	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	1:87:D:ALA:N	3	1.81	0.51	1.57
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	3	1.8	0.48	1.47
(1,53)	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1:38:A:PRO:N	3	1.77	0.56	1.51
(1,272)	1:17:B:TYR:C	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	3	1.76	0.29	1.84
(1,889)	1:78:D:VAL:N	1:78:D:VAL:CA	1:78:D:VAL:C	1:79:D:GLN:N	3	1.74	0.51	1.46
(1,331)	1:50:B:GLN:N	1:50:B:GLN:CA	1:50:B:GLN:C	1:51:B:LEU:N	3	1.7	0.5	1.94
(1,611)	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	1:65:C:THR:N	3	1.7	0.44	1.94
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	3	1.7	0.24	1.61
(1,709)	1:115:C:THR:N	1:115:C:THR:CA	1:115:C:THR:C	1:116:C:SER:N	3	1.66	0.24	1.78
(1,748)	1:136:C:LEU:C	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	3	1.65	0.32	1.53
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	3	1.62	0.6	1.21
(1,419)	1:94:B:MET:N	1:94:B:MET:CA	1:94:B:MET:C	1:95:B:ALA:N	3	1.58	0.47	1.38
(1,727)	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1:126:C:LEU:N	3	1.58	0.42	1.58
(1,835)	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	1:52:D:ALA:N	3	1.49	0.06	1.49
(1,550)	1:32:C:PHE:C	1:33:C:GLN:N	1:33:C:GLN:CA	1:33:C:GLN:C	3	1.48	0.38	1.21
(1,861)	1:64:D:VAL:N	1:64:D:VAL:CA	1:64:D:VAL:C	1:65:D:THR:N	3	1.47	0.28	1.29
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	3	1.47	0.3	1.55
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	3	1.46	0.22	1.58
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	3	1.42	0.21	1.54
(1,510)	1:10:C:THR:C	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	3	1.42	0.2	1.34
(1,643)	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	1:81:C:GLY:N	3	1.35	0.13	1.33
(1,623)	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1:71:C:GLU:N	3	1.34	0.11	1.3
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	3	1.32	0.15	1.3
(1,985)	1:129:D:ALA:N	1:129:D:ALA:CA	1:129:D:ALA:C	1:130:D:PRO:N	3	1.25	0.17	1.26
(1,36)	1:27:A:ASN:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	3	1.23	0.15	1.29
(1,160)	1:91:A:GLY:C	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	2	4.74	0.1	4.74
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	2	3.59	0.37	3.59
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	2	3.46	1.66	3.46
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	2	3.39	2.0	3.39
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	2	3.36	1.39	3.36
(1,222)	1:125:A:GLN:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	2	3.24	0.0	3.24
(1,910)	1:88:D:GLY:C	1:89:D:ILE:N	1:89:D:ILE:CA	1:89:D:ILE:C	2	3.04	0.05	3.04
(1,613)	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	1:66:C:ALA:N	2	2.94	0.72	2.94
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	2	2.84	0.25	2.84
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	2	2.82	0.91	2.82
(1,504)	1:140:B:TYR:C	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	2	2.73	0.44	2.73
(1,337)	1:53:B:ASP:N	1:53:B:ASP:CA	1:53:B:ASP:C	1:54:B:ASP:N	2	2.72	0.07	2.72
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	2	2.71	0.59	2.71
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	2	2.6	1.57	2.6
(1,79)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	2	2.51	0.82	2.51
(1,635)	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1:77:C:GLU:N	2	2.5	0.05	2.5
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	2	2.46	0.09	2.46
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	2	2.46	0.01	2.46
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	2	2.26	0.09	2.26
(1,576)	1:46:C:THR:C	1:47:C:ALA:N	1:47:C:ALA:CA	1:47:C:ALA:C	2	2.24	0.41	2.24

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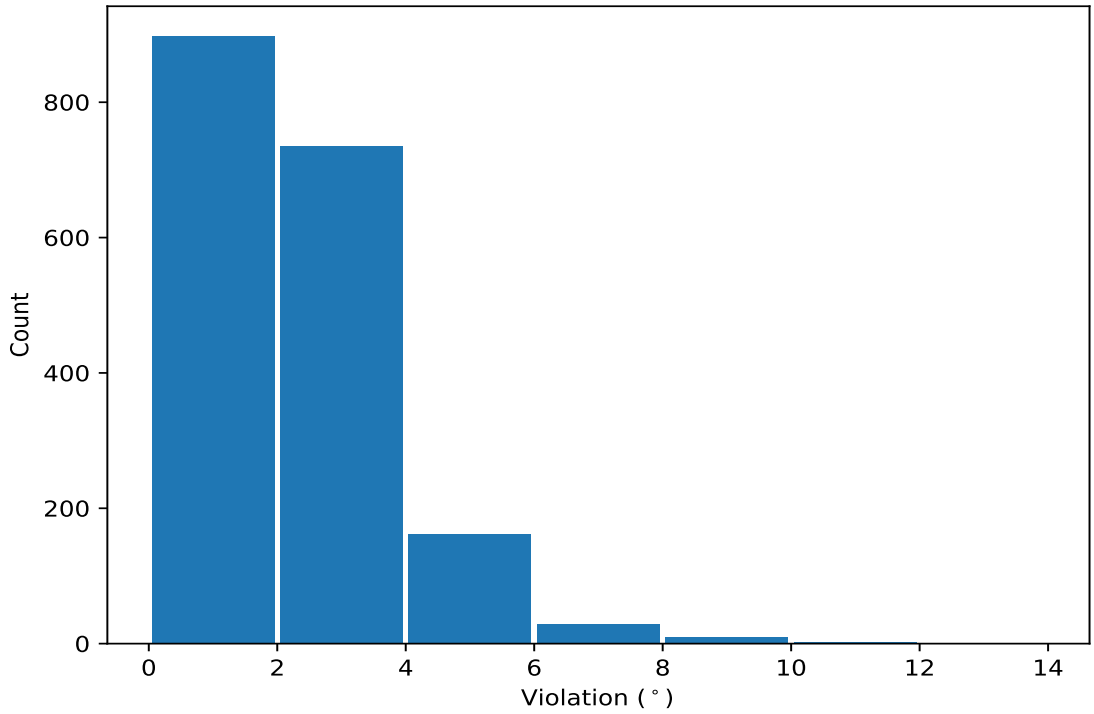
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,787)	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	1:25:D:ALA:N	2	2.23	0.68	2.23
(1,75)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLN:N	2	2.18	0.0	2.18
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	2	2.14	0.82	2.14
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	2	2.12	0.74	2.12
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	2	2.12	1.06	2.12
(1,69)	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1:47:A:ALA:N	2	2.1	0.75	2.1
(1,913)	1:90:D:GLU:N	1:90:D:GLU:CA	1:90:D:GLU:C	1:91:D:GLY:N	2	2.05	0.3	2.05
(1,679)	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	1:99:C:GLY:N	2	2.03	0.89	2.03
(1,786)	1:23:D:PHE:C	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	2	2.0	0.94	2.0
(1,49)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:TRP:N	2	1.99	0.55	1.99
(1,731)	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	1:128:C:LEU:N	2	1.92	0.43	1.92
(1,758)	1:9:D:MET:C	1:10:D:THR:N	1:10:D:THR:CA	1:10:D:THR:C	2	1.85	0.73	1.85
(1,754)	1:139:C:ASN:C	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	2	1.84	0.58	1.84
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	2	1.83	0.11	1.83
(1,158)	1:90:A:GLU:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	2	1.8	0.2	1.8
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	2	1.79	0.14	1.79
(1,770)	1:15:D:ARG:C	1:16:D:ILE:N	1:16:D:ILE:CA	1:16:D:ILE:C	2	1.75	0.7	1.75
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	2	1.72	0.28	1.72
(1,857)	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	1:63:D:THR:N	2	1.71	0.58	1.71
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	2	1.7	0.16	1.7
(1,148)	1:85:A:SER:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	2	1.69	0.03	1.69
(1,287)	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	1:26:B:PRO:N	2	1.68	0.22	1.68
(1,386)	1:77:B:GLU:C	1:78:B:VAL:N	1:78:B:VAL:CA	1:78:B:VAL:C	2	1.63	0.45	1.63
(1,602)	1:59:C:VAL:C	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	2	1.63	0.42	1.63
(1,665)	1:91:C:GLY:N	1:91:C:GLY:CA	1:91:C:GLY:C	1:92:C:THR:N	2	1.59	0.44	1.59
(1,310)	1:39:B:GLU:C	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	2	1.56	0.2	1.56
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	2	1.54	0.21	1.54
(1,685)	1:101:C:TYR:N	1:101:C:TYR:CA	1:101:C:TYR:C	1:102:C:CYS:N	2	1.54	0.46	1.54
(1,94)	1:58:A:VAL:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	2	1.51	0.33	1.51
(1,152)	1:87:A:ALA:C	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	2	1.48	0.06	1.48
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	2	1.46	0.34	1.46
(1,173)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:GLY:N	2	1.44	0.03	1.44
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	2	1.43	0.17	1.43
(1,412)	1:90:B:GLU:C	1:91:B:GLY:N	1:91:B:GLY:CA	1:91:B:GLY:C	2	1.42	0.01	1.42
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	2	1.42	0.34	1.42
(1,788)	1:24:D:GLU:C	1:25:D:ALA:N	1:25:D:ALA:CA	1:25:D:ALA:C	2	1.4	0.02	1.4
(1,906)	1:86:D:ILE:C	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	2	1.39	0.05	1.39
(1,429)	1:99:B:GLY:N	1:99:B:GLY:CA	1:99:B:GLY:C	1:100:B:ALA:N	2	1.27	0.1	1.27
(1,850)	1:58:D:VAL:C	1:59:D:VAL:N	1:59:D:VAL:CA	1:59:D:VAL:C	2	1.25	0.13	1.25
(1,678)	1:97:C:CYS:C	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	2	1.21	0.01	1.21
(1,393)	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1:82:B:GLY:N	2	1.2	0.2	1.2
(1,390)	1:79:B:GLN:C	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	2	1.13	0.01	1.13
(1,856)	1:61:D:ARG:C	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	2	1.04	0.02	1.04

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (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 (°)
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	6	12.15
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	11	11.46
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	19	11.46
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1	9.43
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	18	9.31
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	3	8.71
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	9	8.63
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	15	8.59
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	20	8.26
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	2	8.21
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	7	8.13
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	20	8.1
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	8	7.95
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	17	7.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	6	7.88
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	15	7.68
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	4	7.65
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	8	7.64
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	13	7.47
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	1	7.3
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	7	7.28
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	12	7.26
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	1	7.2
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	16	6.95
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	15	6.95
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	19	6.84
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	10	6.7
(1,415)	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	1:93:B:GLN:N	16	6.66
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	19	6.65
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	11	6.58
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	3	6.4
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	19	6.39
(1,557)	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	1:37:C:GLN:N	3	6.35
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	6	6.33
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	8	6.2
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	3	6.16
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	7	6.14
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	4	6.13
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	7	6.11
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	13	6.11
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	11	6.03
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	6	5.97
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	6	5.94
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	14	5.92
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	8	5.92
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	19	5.9
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	7	5.79
(1,121)	1:72:A:THR:N	1:72:A:THR:CA	1:72:A:THR:C	1:73:A:ALA:N	17	5.77
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	18	5.72
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	14	5.7
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	15	5.65
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	15	5.64
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	17	5.63
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	4	5.58
(1,407)	1:88:B:GLY:N	1:88:B:GLY:CA	1:88:B:GLY:C	1:89:B:ILE:N	17	5.57
(1,38)	1:29:A:PRO:C	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	4	5.57
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	6	5.52
(1,608)	1:62:C:VAL:C	1:63:C:THR:N	1:63:C:THR:CA	1:63:C:THR:C	9	5.5
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	16	5.47
(1,252)	1:141:A:LEU:C	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	9	5.47
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	18	5.47
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	5	5.42
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	16	5.41
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	5	5.4
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	13	5.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	7	5.38
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	13	5.34
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	3	5.34
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	1	5.33
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	12	5.32
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	20	5.32
(1,538)	1:24:C:GLU:C	1:25:C:ALA:N	1:25:C:ALA:CA	1:25:C:ALA:C	6	5.28
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	7	5.24
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	12	5.23
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	7	5.23
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	12	5.22
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	17	5.2
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	5	5.17
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	14	5.16
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	14	5.15
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	7	5.15
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	3	5.14
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	12	5.12
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	8	5.08
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	4	5.08
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	19	5.06
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	9	4.98
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	7	4.97
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	19	4.95
(1,407)	1:88:B:GLY:N	1:88:B:GLY:CA	1:88:B:GLY:C	1:89:B:ILE:N	16	4.95
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	20	4.93
(1,130)	1:76:A:CYS:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	6	4.93
(1,741)	1:133:C:PHE:N	1:133:C:PHE:CA	1:133:C:PHE:C	1:134:C:ASP:N	10	4.92
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	9	4.92
(1,728)	1:125:C:GLN:C	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	9	4.9
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	15	4.9
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	4	4.88
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	3	4.87
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	1	4.87
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	11	4.87
(1,160)	1:91:A:GLY:C	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	16	4.84
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	14	4.84
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	15	4.83
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	7	4.83
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	14	4.83
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	6	4.8
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	11	4.78
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	9	4.77
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	10	4.76
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	4	4.75
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	9	4.74
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	8	4.74
(1,321)	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1:46:B:THR:N	14	4.71
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	8	4.7
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	9	4.68
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	11	4.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	1	4.67
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	9	4.66
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	18	4.65
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	2	4.64
(1,160)	1:91:A:GLY:C	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	19	4.64
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	4	4.61
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	13	4.57
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	2	4.57
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	6	4.57
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	5	4.55
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	10	4.54
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	5	4.54
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	2	4.54
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	7	4.54
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	10	4.53
(1,887)	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	1:78:D:VAL:N	11	4.53
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	8	4.53
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	18	4.52
(1,728)	1:125:C:GLN:C	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	6	4.52
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	17	4.52
(1,224)	1:126:A:LEU:C	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	15	4.52
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	12	4.49
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	10	4.49
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	1	4.48
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	7	4.46
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	19	4.46
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	13	4.45
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	20	4.43
(1,17)	1:17:A:TYR:N	1:17:A:TYR:CA	1:17:A:TYR:C	1:18:A:THR:N	10	4.42
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	20	4.41
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	3	4.38
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	12	4.38
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	18	4.37
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	7	4.37
(1,258)	1:10:B:THR:C	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	18	4.36
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	4	4.34
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	15	4.34
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	6	4.34
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	4	4.33
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	5	4.33
(1,815)	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	1:42:D:LEU:N	13	4.32
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	10	4.32
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	3	4.32
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	4	4.31
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	17	4.3
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	7	4.3
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	11	4.3
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	3	4.29
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	1	4.29
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	8	4.27
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	9	4.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	10	4.27
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	20	4.27
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	12	4.26
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	8	4.25
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	9	4.23
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	2	4.23
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	6	4.23
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	3	4.21
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	12	4.2
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	10	4.2
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	16	4.18
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	1	4.18
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	8	4.15
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	13	4.15
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	12	4.14
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	13	4.14
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	3	4.13
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	6	4.13
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	9	4.12
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	15	4.12
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	6	4.11
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	9	4.11
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	11	4.11
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	18	4.09
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	9	4.08
(1,978)	1:125:D:GLN:C	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	13	4.07
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	17	4.07
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	5	4.07
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	3	4.07
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	2	4.06
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	19	4.06
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	1	4.03
(1,104)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	14	4.01
(1,37)	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1:29:A:PRO:N	2	4.01
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	8	4.0
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	15	4.0
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	5	3.99
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	7	3.98
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	5	3.97
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	9	3.97
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	18	3.97
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	17	3.96
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	7	3.96
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	20	3.96
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	20	3.95
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	5	3.95
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	12	3.93
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	18	3.93
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	12	3.92
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	16	3.92
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	16	3.92

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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	7	3.9
(1,523)	1:17:C:TYR:N	1:17:C:TYR:CA	1:17:C:TYR:C	1:18:C:THR:N	14	3.89
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	15	3.88
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	20	3.87
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	11	3.87
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	16	3.87
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	13	3.84
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	20	3.83
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	5	3.82
(1,612)	1:64:C:VAL:C	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	17	3.82
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	8	3.82
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	13	3.82
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	8	3.81
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	6	3.81
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1	3.81
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	14	3.8
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	19	3.8
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	18	3.77
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	15	3.77
(1,570)	1:43:C:ASP:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	16	3.77
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	15	3.77
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	2	3.76
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	6	3.76
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	8	3.75
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	19	3.74
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	1	3.74
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	3	3.74
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	7	3.73
(1,108)	1:65:A:THR:C	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	7	3.73
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	6	3.72
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	9	3.7
(1,321)	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1:46:B:THR:N	19	3.7
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	6	3.7
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	3	3.68
(1,613)	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	1:66:C:ALA:N	8	3.67
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	17	3.67
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	7	3.66
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	18	3.66
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	11	3.63
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	15	3.63
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	3	3.63
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	16	3.62
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	10	3.61
(1,321)	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1:46:B:THR:N	7	3.61
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	12	3.61
(1,311)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:LYS:N	4	3.59
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	18	3.59
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	1	3.59
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	15	3.58
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	5	3.57
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	16	3.55

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	15	3.55
(1,130)	1:76:A:CYS:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	14	3.55
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	17	3.55
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	11	3.54
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	12	3.54
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	12	3.54
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	7	3.54
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	14	3.54
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	2	3.53
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	17	3.53
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	3	3.53
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	9	3.52
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	14	3.52
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	6	3.52
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	7	3.51
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	3	3.51
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	1	3.5
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	12	3.5
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	2	3.49
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	4	3.48
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	4	3.47
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	4	3.46
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	17	3.46
(1,219)	1:123:A:PHE:N	1:123:A:PHE:CA	1:123:A:PHE:C	1:124:A:PRO:N	1	3.46
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	3	3.45
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	10	3.45
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	9	3.44
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	17	3.44
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	2	3.44
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	20	3.44
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	4	3.43
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	20	3.43
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	2	3.42
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	7	3.42
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	9	3.41
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	6	3.41
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	19	3.41
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	17	3.39
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	10	3.38
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1	3.37
(1,362)	1:65:B:THR:C	1:66:B:ALA:N	1:66:B:ALA:CA	1:66:B:ALA:C	14	3.36
(1,104)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	13	3.36
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	4	3.35
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	2	3.35
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	12	3.35
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	16	3.34
(1,372)	1:70:B:GLU:C	1:71:B:GLU:N	1:71:B:GLU:CA	1:71:B:GLU:C	1	3.34
(1,79)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	8	3.34
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	15	3.33
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	16	3.33
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	2	3.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	6	3.31
(1,163)	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	1:94:A:MET:N	19	3.31
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	2	3.3
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	17	3.3
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	14	3.3
(1,486)	1:131:B:VAL:C	1:132:B:ASN:N	1:132:B:ASN:CA	1:132:B:ASN:C	15	3.29
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	16	3.28
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	12	3.28
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	2	3.27
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	4	3.27
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	18	3.26
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	10	3.26
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	2	3.26
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1	3.25
(1,322)	1:45:B:ASP:C	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	20	3.25
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	1	3.25
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	16	3.24
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	8	3.24
(1,222)	1:125:A:GLN:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	10	3.24
(1,222)	1:125:A:GLN:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	15	3.24
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	15	3.23
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	9	3.23
(1,751)	1:138:C:MET:N	1:138:C:MET:CA	1:138:C:MET:C	1:139:C:ASN:N	6	3.22
(1,621)	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	1:70:C:GLU:N	12	3.22
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	12	3.21
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	8	3.21
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	2	3.21
(1,383)	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	1:77:B:GLU:N	12	3.21
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	10	3.21
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	10	3.21
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	10	3.21
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	8	3.2
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	17	3.2
(1,324)	1:46:B:THR:C	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	3	3.2
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	15	3.19
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	7	3.19
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	15	3.18
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	18	3.18
(1,176)	1:99:A:GLY:C	1:100:A:ALA:N	1:100:A:ALA:CA	1:100:A:ALA:C	17	3.18
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	18	3.17
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	4	3.17
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	7	3.17
(1,504)	1:140:B:TYR:C	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	8	3.17
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	14	3.17
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	7	3.17
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	9	3.17
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	2	3.16
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	19	3.16
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	20	3.15
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	13	3.15
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	2	3.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,70)	1:46:A:THR:C	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	18	3.14
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	17	3.13
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	20	3.13
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	14	3.13
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	20	3.13
(1,815)	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	1:42:D:LEU:N	8	3.12
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	20	3.12
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	12	3.11
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	1	3.11
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	16	3.11
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	5	3.1
(1,910)	1:88:D:GLY:C	1:89:D:ILE:N	1:89:D:ILE:CA	1:89:D:ILE:C	12	3.1
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	10	3.1
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	20	3.1
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	2	3.09
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	1	3.09
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	4	3.09
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	7	3.09
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	18	3.09
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	5	3.09
(1,660)	1:88:C:GLY:C	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	6	3.08
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	15	3.08
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	3	3.08
(1,645)	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	1:82:C:GLY:N	18	3.07
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	4	3.07
(1,411)	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	1:91:B:GLY:N	15	3.06
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	17	3.06
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	17	3.06
(1,17)	1:17:A:TYR:N	1:17:A:TYR:CA	1:17:A:TYR:C	1:18:A:THR:N	20	3.06
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	1	3.05
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1	3.05
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	12	3.05
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	12	3.04
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	2	3.04
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	4	3.03
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1	3.03
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	19	3.03
(1,823)	1:45:D:ASP:N	1:45:D:ASP:CA	1:45:D:ASP:C	1:46:D:THR:N	16	3.02
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	10	3.02
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	8	3.02
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	13	3.01
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	13	3.01
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	16	3.01
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	17	3.01
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	20	3.01
(1,975)	1:123:D:PHE:N	1:123:D:PHE:CA	1:123:D:PHE:C	1:124:D:PRO:N	14	3.0
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	3	3.0
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	20	3.0
(1,22)	1:19:A:LYS:C	1:20:A:ASP:N	1:20:A:ASP:CA	1:20:A:ASP:C	5	3.0
(1,910)	1:88:D:GLY:C	1:89:D:ILE:N	1:89:D:ILE:CA	1:89:D:ILE:C	7	2.99
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	15	2.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	18	2.99
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	13	2.99
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	20	2.99
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	19	2.99
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	6	2.99
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	1	2.98
(1,579)	1:48:C:SER:N	1:48:C:SER:CA	1:48:C:SER:C	1:49:C:SER:N	17	2.98
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	12	2.98
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	16	2.97
(1,538)	1:24:C:GLU:C	1:25:C:ALA:N	1:25:C:ALA:CA	1:25:C:ALA:C	16	2.96
(1,476)	1:125:B:GLN:C	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	18	2.96
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	2	2.96
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	18	2.96
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	12	2.95
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	10	2.95
(1,786)	1:23:D:PHE:C	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	13	2.94
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	18	2.93
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	16	2.92
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	1	2.92
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	14	2.92
(1,679)	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	1:99:C:GLY:N	8	2.92
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	14	2.92
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	7	2.92
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	11	2.91
(1,787)	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	1:25:D:ALA:N	15	2.91
(1,311)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:LYS:N	14	2.91
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	8	2.91
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	5	2.91
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	12	2.91
(1,645)	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	1:82:C:GLY:N	12	2.9
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	11	2.9
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	13	2.9
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	20	2.9
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	20	2.89
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	1	2.89
(1,180)	1:101:A:TYR:C	1:102:A:CYS:N	1:102:A:CYS:CA	1:102:A:CYS:C	17	2.89
(1,885)	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	1:77:D:GLU:N	5	2.88
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	19	2.88
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1	2.88
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	12	2.88
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	20	2.88
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	3	2.87
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1	2.87
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	3	2.87
(1,118)	1:70:A:GLU:C	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	12	2.87
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	1	2.86
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	16	2.86
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	8	2.85
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	4	2.85
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	15	2.85
(1,69)	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1:47:A:ALA:N	14	2.85

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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	2	2.84
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	1	2.84
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	5	2.84
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	20	2.84
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	11	2.84
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	20	2.84
(1,820)	1:43:D:ASP:C	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	15	2.83
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	18	2.82
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	9	2.82
(1,511)	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	1:12:C:GLN:N	10	2.82
(1,415)	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	1:93:B:GLN:N	3	2.82
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	8	2.81
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	18	2.81
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	14	2.81
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	4	2.81
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	8	2.81
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	16	2.8
(1,571)	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	1:45:C:ASP:N	10	2.8
(1,337)	1:53:B:ASP:N	1:53:B:ASP:CA	1:53:B:ASP:C	1:54:B:ASP:N	17	2.8
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	4	2.8
(1,739)	1:132:C:ASN:N	1:132:C:ASN:CA	1:132:C:ASN:C	1:133:C:PHE:N	20	2.79
(1,561)	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	1:40:C:VAL:N	14	2.79
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	17	2.79
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	20	2.79
(1,5)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:GLN:N	2	2.79
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1	2.78
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	19	2.78
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	8	2.78
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	15	2.77
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	8	2.75
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	7	2.75
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	13	2.75
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	3	2.75
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	20	2.75
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	3	2.75
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	5	2.75
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	2	2.75
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	7	2.74
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	11	2.74
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	13	2.74
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	7	2.74
(1,70)	1:46:A:THR:C	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1	2.74
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	20	2.73
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	19	2.72
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	5	2.71
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	8	2.7
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	14	2.7
(1,769)	1:15:D:ARG:N	1:15:D:ARG:CA	1:15:D:ARG:C	1:16:D:ILE:N	3	2.7
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	5	2.7
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	11	2.7
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	17	2.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,109)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:SER:N	2	2.7
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	9	2.7
(1,983)	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	1:129:D:ALA:N	4	2.69
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	9	2.69
(1,761)	1:11:D:PHE:N	1:11:D:PHE:CA	1:11:D:PHE:C	1:12:D:GLN:N	20	2.69
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	2	2.69
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	20	2.69
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	8	2.69
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1	2.69
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	4	2.68
(1,663)	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	1:91:C:GLY:N	6	2.68
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	13	2.68
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	10	2.68
(1,523)	1:17:C:TYR:N	1:17:C:TYR:CA	1:17:C:TYR:C	1:18:C:THR:N	10	2.68
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	1	2.68
(1,252)	1:141:A:LEU:C	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	19	2.68
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	8	2.68
(1,223)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:ASN:N	10	2.68
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	14	2.68
(1,101)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:THR:N	20	2.68
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	8	2.67
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	16	2.67
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	15	2.67
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	7	2.67
(1,119)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:THR:N	17	2.67
(1,576)	1:46:C:THR:C	1:47:C:ALA:N	1:47:C:ALA:CA	1:47:C:ALA:C	9	2.65
(1,337)	1:53:B:ASP:N	1:53:B:ASP:CA	1:53:B:ASP:C	1:54:B:ASP:N	16	2.65
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	12	2.64
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	9	2.63
(1,756)	1:8:D:GLU:C	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	10	2.63
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	16	2.63
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	20	2.63
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	11	2.63
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	19	2.63
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	17	2.62
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	6	2.62
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	20	2.62
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	16	2.62
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	16	2.62
(1,95)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:LEU:N	9	2.62
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	14	2.61
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	8	2.61
(1,880)	1:73:D:ALA:C	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	3	2.6
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	4	2.6
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	14	2.6
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	2	2.59
(1,758)	1:9:D:MET:C	1:10:D:THR:N	1:10:D:THR:CA	1:10:D:THR:C	14	2.58
(1,661)	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	1:90:C:GLU:N	12	2.58
(1,309)	1:39:B:GLU:N	1:39:B:GLU:CA	1:39:B:GLU:C	1:40:B:VAL:N	17	2.58
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	15	2.58
(1,916)	1:91:D:GLY:C	1:92:D:THR:N	1:92:D:THR:CA	1:92:D:THR:C	8	2.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,883)	1:75:D:LEU:N	1:75:D:LEU:CA	1:75:D:LEU:C	1:76:D:CYS:N	19	2.57
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	13	2.57
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	17	2.57
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	2	2.56
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	6	2.56
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	8	2.56
(1,109)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:SER:N	16	2.56
(1,96)	1:59:A:VAL:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	18	2.56
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	14	2.56
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	18	2.55
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	10	2.55
(1,635)	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1:77:C:GLU:N	6	2.55
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	12	2.55
(1,520)	1:15:C:ARG:C	1:16:C:ILE:N	1:16:C:ILE:CA	1:16:C:ILE:C	20	2.55
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	20	2.55
(1,53)	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1:38:A:PRO:N	9	2.55
(1,819)	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	1:44:D:LEU:N	10	2.54
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	13	2.54
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	18	2.54
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	13	2.54
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	20	2.54
(1,49)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:TRP:N	13	2.54
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	20	2.53
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	20	2.53
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	9	2.53
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	7	2.53
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	12	2.52
(1,645)	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	1:82:C:GLY:N	7	2.52
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	9	2.52
(1,495)	1:136:B:LEU:N	1:136:B:LEU:CA	1:136:B:LEU:C	1:137:B:PHE:N	13	2.52
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	14	2.52
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	8	2.52
(1,905)	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	1:87:D:ALA:N	6	2.51
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	11	2.51
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	15	2.5
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	11	2.5
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	5	2.5
(1,77)	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	1:51:A:LEU:N	3	2.5
(1,70)	1:46:A:THR:C	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	11	2.5
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	17	2.5
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	6	2.49
(1,979)	1:126:D:LEU:N	1:126:D:LEU:CA	1:126:D:LEU:C	1:127:D:ASN:N	1	2.49
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	20	2.49
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	10	2.49
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	20	2.49
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	14	2.49
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	6	2.49
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	8	2.49
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	14	2.49
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	15	2.48
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	6	2.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	13	2.48
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	11	2.48
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	7	2.48
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	14	2.48
(1,728)	1:125:C:GLN:C	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	12	2.48
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	17	2.47
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	9	2.47
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	1	2.47
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	2	2.47
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	12	2.47
(1,881)	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	1:75:D:LEU:N	20	2.46
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	7	2.46
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	17	2.45
(1,889)	1:78:D:VAL:N	1:78:D:VAL:CA	1:78:D:VAL:C	1:79:D:GLN:N	11	2.45
(1,813)	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	1:41:D:LYS:N	14	2.45
(1,770)	1:15:D:ARG:C	1:16:D:ILE:N	1:16:D:ILE:CA	1:16:D:ILE:C	12	2.45
(1,635)	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1:77:C:GLU:N	17	2.45
(1,372)	1:70:B:GLU:C	1:71:B:GLU:N	1:71:B:GLU:CA	1:71:B:GLU:C	15	2.45
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	20	2.45
(1,105)	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1:65:A:THR:N	11	2.45
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	7	2.44
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	5	2.44
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	3	2.44
(1,95)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:LEU:N	8	2.44
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	13	2.43
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	10	2.43
(1,761)	1:11:D:PHE:N	1:11:D:PHE:CA	1:11:D:PHE:C	1:12:D:GLN:N	4	2.42
(1,754)	1:139:C:ASN:C	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	5	2.41
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	18	2.41
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	10	2.41
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	11	2.41
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	4	2.4
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	14	2.4
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	11	2.4
(1,655)	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	1:87:C:ALA:N	7	2.4
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	5	2.4
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	19	2.4
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	13	2.4
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	19	2.4
(1,660)	1:88:C:GLY:C	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	10	2.39
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	16	2.39
(1,108)	1:65:A:THR:C	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	16	2.39
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	6	2.39
(1,67)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:THR:N	6	2.39
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	18	2.38
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	2	2.38
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	16	2.38
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	3	2.38
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	11	2.38
(1,45)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:LYS:N	12	2.38
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	9	2.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,901)	1:84:D:PHE:N	1:84:D:PHE:CA	1:84:D:PHE:C	1:85:D:SER:N	4	2.37
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	1	2.37
(1,583)	1:50:C:GLN:N	1:50:C:GLN:CA	1:50:C:GLN:C	1:51:C:LEU:N	5	2.37
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	13	2.37
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	12	2.37
(1,252)	1:141:A:LEU:C	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	14	2.37
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	15	2.37
(1,913)	1:90:D:GLU:N	1:90:D:GLU:CA	1:90:D:GLU:C	1:91:D:GLY:N	14	2.36
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	17	2.36
(1,819)	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	1:44:D:LEU:N	20	2.36
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	4	2.36
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	16	2.36
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	20	2.36
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	16	2.36
(1,101)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:THR:N	9	2.36
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	14	2.36
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	8	2.35
(1,731)	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	1:128:C:LEU:N	16	2.35
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	20	2.35
(1,610)	1:63:C:THR:C	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	8	2.35
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	3	2.35
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	18	2.35
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	4	2.35
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	12	2.35
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	19	2.35
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	7	2.35
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	2	2.34
(1,224)	1:126:A:LEU:C	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	14	2.34
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	16	2.34
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	7	2.34
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	7	2.34
(1,655)	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	1:87:C:ALA:N	12	2.33
(1,70)	1:46:A:THR:C	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	4	2.33
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	11	2.33
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	11	2.33
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	4	2.32
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	5	2.32
(1,403)	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1:87:B:ALA:N	10	2.32
(1,362)	1:65:B:THR:C	1:66:B:ALA:N	1:66:B:ALA:CA	1:66:B:ALA:C	8	2.32
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	7	2.32
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	3	2.31
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	1	2.31
(1,551)	1:33:C:GLN:N	1:33:C:GLN:CA	1:33:C:GLN:C	1:34:C:LYS:N	12	2.31
(1,415)	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	1:93:B:GLN:N	11	2.31
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	17	2.31
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	15	2.3
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	7	2.3
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	7	2.3
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	16	2.3
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	18	2.3
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	14	2.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,119)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:THR:N	20	2.3
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	3	2.29
(1,857)	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	1:63:D:THR:N	11	2.29
(1,504)	1:140:B:TYR:C	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1	2.29
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	15	2.29
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	4	2.29
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	10	2.28
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	13	2.28
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	17	2.28
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	3	2.28
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	8	2.28
(1,264)	1:13:B:ILE:C	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	12	2.28
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	8	2.28
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	16	2.27
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	6	2.27
(1,224)	1:126:A:LEU:C	1:127:A:ASN:N	1:127:A:ASN:CA	1:127:A:ASN:C	1	2.27
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	20	2.27
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	12	2.27
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	18	2.26
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	2	2.26
(1,644)	1:80:C:GLN:C	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	12	2.26
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	3	2.26
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	9	2.25
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	14	2.24
(1,316)	1:42:B:LEU:C	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	12	2.24
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	19	2.24
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	2	2.24
(1,60)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	14	2.24
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	20	2.23
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	15	2.23
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	6	2.23
(1,419)	1:94:B:MET:N	1:94:B:MET:CA	1:94:B:MET:C	1:95:B:ALA:N	14	2.23
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	12	2.23
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	1	2.23
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	19	2.23
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	6	2.23
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	3	2.22
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	7	2.22
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	4	2.22
(1,613)	1:65:C:THR:N	1:65:C:THR:CA	1:65:C:THR:C	1:66:C:ALA:N	2	2.22
(1,324)	1:46:B:THR:C	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	10	2.22
(1,983)	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	1:129:D:ALA:N	12	2.21
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	16	2.21
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	3	2.21
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	9	2.21
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	1	2.21
(1,321)	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1:46:B:THR:N	20	2.21
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	20	2.21
(1,104)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	11	2.21
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1	2.21
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	11	2.2

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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	19	2.2
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	16	2.2
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	3	2.2
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	12	2.2
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	13	2.2
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	11	2.2
(1,104)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	7	2.2
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	17	2.19
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	16	2.19
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	16	2.19
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	5	2.19
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	12	2.19
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	5	2.19
(1,75)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLN:N	16	2.19
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	20	2.18
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	8	2.18
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	20	2.18
(1,104)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1	2.18
(1,75)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLN:N	10	2.18
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	16	2.17
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	19	2.17
(1,769)	1:15:D:ARG:N	1:15:D:ARG:CA	1:15:D:ARG:C	1:16:D:ILE:N	17	2.17
(1,645)	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	1:82:C:GLY:N	2	2.17
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	13	2.17
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	7	2.17
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	17	2.17
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	3	2.17
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	3	2.16
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	13	2.16
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	8	2.16
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	9	2.16
(1,489)	1:133:B:PHE:N	1:133:B:PHE:CA	1:133:B:PHE:C	1:134:B:ASP:N	13	2.16
(1,479)	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	1:128:B:LEU:N	15	2.16
(1,22)	1:19:A:LYS:C	1:20:A:ASP:N	1:20:A:ASP:CA	1:20:A:ASP:C	13	2.16
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	1	2.16
(1,822)	1:44:D:LEU:C	1:45:D:ASP:N	1:45:D:ASP:CA	1:45:D:ASP:C	4	2.15
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	6	2.15
(1,559)	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	1:38:C:PRO:N	19	2.15
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	10	2.15
(1,331)	1:50:B:GLN:N	1:50:B:GLN:CA	1:50:B:GLN:C	1:51:B:LEU:N	4	2.15
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	19	2.15
(1,229)	1:129:A:ALA:N	1:129:A:ALA:CA	1:129:A:ALA:C	1:130:A:PRO:N	7	2.15
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	6	2.15
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	5	2.15
(1,846)	1:56:D:TYR:C	1:57:D:GLU:N	1:57:D:GLU:CA	1:57:D:GLU:C	16	2.14
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	10	2.14
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	10	2.14
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	7	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
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	14	2.13
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	12	2.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	17	2.13
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	18	2.13
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	3	2.13
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	3	2.13
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	14	2.12
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	5	2.12
(1,559)	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	1:38:C:PRO:N	16	2.12
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	6	2.12
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	11	2.12
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	4	2.12
(1,260)	1:11:B:PHE:C	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	18	2.12
(1,155)	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	1:90:A:GLU:N	15	2.12
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	17	2.12
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	13	2.11
(1,597)	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	1:58:C:VAL:N	3	2.11
(1,403)	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1:87:B:ALA:N	19	2.11
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	16	2.11
(1,333)	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	1:52:B:ALA:N	1	2.11
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	6	2.11
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	17	2.11
(1,101)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:THR:N	1	2.11
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	2	2.1
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	11	2.1
(1,901)	1:84:D:PHE:N	1:84:D:PHE:CA	1:84:D:PHE:C	1:85:D:SER:N	6	2.1
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	11	2.1
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	7	2.1
(1,727)	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1:126:C:LEU:N	9	2.1
(1,645)	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	1:82:C:GLY:N	15	2.1
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	18	2.1
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	17	2.1
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	11	2.1
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	14	2.1
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	9	2.1
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	12	2.09
(1,610)	1:63:C:THR:C	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	20	2.09
(1,386)	1:77:B:GLU:C	1:78:B:VAL:N	1:78:B:VAL:CA	1:78:B:VAL:C	12	2.09
(1,321)	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1:46:B:THR:N	8	2.09
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	15	2.09
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	14	2.09
(1,748)	1:136:C:LEU:C	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	2	2.08
(1,644)	1:80:C:GLN:C	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	13	2.08
(1,611)	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	1:65:C:THR:N	8	2.08
(1,401)	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	1:86:B:ILE:N	15	2.08
(1,315)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:ASP:N	15	2.08
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	10	2.08
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	10	2.07
(1,489)	1:133:B:PHE:N	1:133:B:PHE:CA	1:133:B:PHE:C	1:134:B:ASP:N	4	2.07
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	6	2.07
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	19	2.07
(1,365)	1:67:B:SER:N	1:67:B:SER:CA	1:67:B:SER:C	1:68:B:LEU:N	7	2.07
(1,272)	1:17:B:TYR:C	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	3	2.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	19	2.07
(1,104)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	20	2.07
(1,488)	1:132:B:ASN:C	1:133:B:PHE:N	1:133:B:PHE:CA	1:133:B:PHE:C	17	2.06
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	11	2.06
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	1	2.05
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	19	2.05
(1,644)	1:80:C:GLN:C	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	20	2.05
(1,602)	1:59:C:VAL:C	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	14	2.05
(1,528)	1:19:C:LYS:C	1:20:C:ASP:N	1:20:C:ASP:CA	1:20:C:ASP:C	20	2.05
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	10	2.05
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	13	2.05
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	9	2.05
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	8	2.04
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	11	2.04
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	17	2.04
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	13	2.04
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	16	2.04
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	2	2.04
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	17	2.04
(1,407)	1:88:B:GLY:N	1:88:B:GLY:CA	1:88:B:GLY:C	1:89:B:ILE:N	19	2.04
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	19	2.04
(1,262)	1:12:B:GLN:C	1:13:B:ILE:N	1:13:B:ILE:CA	1:13:B:ILE:C	11	2.04
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	19	2.03
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	11	2.03
(1,665)	1:91:C:GLY:N	1:91:C:GLY:CA	1:91:C:GLY:C	1:92:C:THR:N	6	2.03
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	9	2.03
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	18	2.03
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	14	2.03
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	4	2.03
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	11	2.03
(1,819)	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	1:44:D:LEU:N	9	2.02
(1,550)	1:32:C:PHE:C	1:33:C:GLN:N	1:33:C:GLN:CA	1:33:C:GLN:C	4	2.02
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	5	2.02
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1	2.02
(1,37)	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1:29:A:PRO:N	11	2.02
(1,880)	1:73:D:ALA:C	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	16	2.01
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	20	2.01
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	1	2.01
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	11	2.01
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	20	2.01
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	20	2.01
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	19	2.01
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	2	2.01
(1,158)	1:90:A:GLU:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	13	2.01
(1,102)	1:62:A:VAL:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	2	2.01
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	14	2.01
(1,17)	1:17:A:TYR:N	1:17:A:TYR:CA	1:17:A:TYR:C	1:18:A:THR:N	6	2.01
(1,974)	1:122:D:THR:C	1:123:D:PHE:N	1:123:D:PHE:CA	1:123:D:PHE:C	1	2.0
(1,685)	1:101:C:TYR:N	1:101:C:TYR:CA	1:101:C:TYR:C	1:102:C:CYS:N	16	2.0
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	13	2.0
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	7	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,324)	1:46:B:THR:C	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	12	2.0
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1	2.0
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	15	2.0
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	11	2.0
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	17	2.0
(1,17)	1:17:A:TYR:N	1:17:A:TYR:CA	1:17:A:TYR:C	1:18:A:THR:N	19	2.0
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	5	1.99
(1,523)	1:17:C:TYR:N	1:17:C:TYR:CA	1:17:C:TYR:C	1:18:C:THR:N	15	1.99
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	16	1.99
(1,371)	1:70:B:GLU:N	1:70:B:GLU:CA	1:70:B:GLU:C	1:71:B:GLU:N	19	1.99
(1,50)	1:35:A:ASP:C	1:36:A:TRP:N	1:36:A:TRP:CA	1:36:A:TRP:C	16	1.99
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	2	1.98
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	19	1.98
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	4	1.98
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	17	1.98
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	9	1.98
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	3	1.98
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	2	1.97
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	17	1.97
(1,605)	1:61:C:ARG:N	1:61:C:ARG:CA	1:61:C:ARG:C	1:62:C:VAL:N	15	1.97
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	6	1.97
(1,570)	1:43:C:ASP:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	19	1.97
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	1	1.97
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	17	1.97
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	12	1.97
(1,974)	1:122:D:THR:C	1:123:D:PHE:N	1:123:D:PHE:CA	1:123:D:PHE:C	14	1.96
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	15	1.96
(1,724)	1:122:C:THR:C	1:123:C:PHE:N	1:123:C:PHE:CA	1:123:C:PHE:C	4	1.96
(1,615)	1:66:C:ALA:N	1:66:C:ALA:CA	1:66:C:ALA:C	1:67:C:SER:N	6	1.96
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	14	1.96
(1,410)	1:89:B:ILE:C	1:90:B:GLU:N	1:90:B:GLU:CA	1:90:B:GLU:C	11	1.96
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	11	1.96
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	1	1.96
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	17	1.95
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	4	1.95
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	19	1.95
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	8	1.95
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	19	1.95
(1,22)	1:19:A:LYS:C	1:20:A:ASP:N	1:20:A:ASP:CA	1:20:A:ASP:C	7	1.95
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	3	1.94
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	18	1.94
(1,611)	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	1:65:C:THR:N	17	1.94
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	13	1.94
(1,494)	1:135:B:ALA:C	1:136:B:LEU:N	1:136:B:LEU:CA	1:136:B:LEU:C	13	1.94
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	6	1.94
(1,331)	1:50:B:GLN:N	1:50:B:GLN:CA	1:50:B:GLN:C	1:51:B:LEU:N	2	1.94
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	3	1.94
(1,305)	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1:37:B:GLN:N	15	1.94
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	6	1.94
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	7	1.93
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	12	1.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	6	1.93
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	17	1.93
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	3	1.93
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	8	1.93
(1,315)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:ASP:N	5	1.93
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	7	1.93
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	3	1.92
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	8	1.92
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	9	1.92
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	5	1.92
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	20	1.92
(1,275)	1:19:B:LYS:N	1:19:B:LYS:CA	1:19:B:LYS:C	1:20:B:ASP:N	13	1.92
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	4	1.92
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	17	1.91
(1,729)	1:126:C:LEU:N	1:126:C:LEU:CA	1:126:C:LEU:C	1:127:C:ASN:N	8	1.91
(1,324)	1:46:B:THR:C	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	11	1.91
(1,304)	1:35:B:ASP:C	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	9	1.91
(1,287)	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	1:26:B:PRO:N	14	1.91
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	10	1.91
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	3	1.9
(1,901)	1:84:D:PHE:N	1:84:D:PHE:CA	1:84:D:PHE:C	1:85:D:SER:N	11	1.9
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	8	1.9
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	17	1.9
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	11	1.9
(1,274)	1:18:B:THR:C	1:19:B:LYS:N	1:19:B:LYS:CA	1:19:B:LYS:C	12	1.9
(1,109)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:SER:N	11	1.9
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	6	1.9
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	12	1.9
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	10	1.9
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	13	1.89
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	11	1.89
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	14	1.89
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	16	1.89
(1,218)	1:122:A:THR:C	1:123:A:PHE:N	1:123:A:PHE:CA	1:123:A:PHE:C	15	1.89
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	17	1.89
(1,1009)	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	1:143:D:GLN:N	16	1.88
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	19	1.88
(1,709)	1:115:C:THR:N	1:115:C:THR:CA	1:115:C:THR:C	1:116:C:SER:N	19	1.88
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	19	1.88
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	6	1.88
(1,312)	1:40:B:VAL:C	1:41:B:LYS:N	1:41:B:LYS:CA	1:41:B:LYS:C	8	1.88
(1,299)	1:33:B:GLN:N	1:33:B:GLN:CA	1:33:B:GLN:C	1:34:B:LYS:N	3	1.88
(1,38)	1:29:A:PRO:C	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	20	1.88
(1,999)	1:137:D:PHE:N	1:137:D:PHE:CA	1:137:D:PHE:C	1:138:D:MET:N	16	1.87
(1,861)	1:64:D:VAL:N	1:64:D:VAL:CA	1:64:D:VAL:C	1:65:D:THR:N	13	1.87
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	4	1.87
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	7	1.87
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	13	1.87
(1,119)	1:71:A:GLU:N	1:71:A:GLU:CA	1:71:A:GLU:C	1:72:A:THR:N	18	1.87
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	6	1.87
(1,101)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:THR:N	12	1.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:24:A:GLU:C	1:25:A:ALA:N	1:25:A:ALA:CA	1:25:A:ALA:C	12	1.87
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	8	1.86
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1	1.86
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	17	1.86
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	13	1.86
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	15	1.86
(1,741)	1:133:C:PHE:N	1:133:C:PHE:CA	1:133:C:PHE:C	1:134:C:ASP:N	13	1.85
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	1	1.85
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	11	1.85
(1,62)	1:42:A:LEU:C	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	20	1.85
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	4	1.84
(1,596)	1:56:C:TYR:C	1:57:C:GLU:N	1:57:C:GLU:CA	1:57:C:GLU:C	8	1.84
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	9	1.84
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	17	1.84
(1,354)	1:61:B:ARG:C	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	12	1.84
(1,272)	1:17:B:TYR:C	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	18	1.84
(1,115)	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	1:70:A:GLU:N	16	1.84
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	2	1.84
(1,94)	1:58:A:VAL:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	9	1.84
(1,983)	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	1:129:D:ALA:N	6	1.83
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	4	1.83
(1,576)	1:46:C:THR:C	1:47:C:ALA:N	1:47:C:ALA:CA	1:47:C:ALA:C	17	1.83
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	14	1.83
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	18	1.83
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	9	1.83
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	13	1.82
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	4	1.82
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	8	1.82
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	7	1.82
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	15	1.82
(1,560)	1:38:C:PRO:C	1:39:C:GLU:N	1:39:C:GLU:CA	1:39:C:GLU:C	1	1.82
(1,362)	1:65:B:THR:C	1:66:B:ALA:N	1:66:B:ALA:CA	1:66:B:ALA:C	10	1.82
(1,92)	1:57:A:GLU:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	3	1.82
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	7	1.82
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	15	1.81
(1,880)	1:73:D:ALA:C	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	4	1.81
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	14	1.81
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	4	1.81
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	13	1.81
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	5	1.81
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	10	1.81
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	18	1.81
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	17	1.81
(1,237)	1:134:A:ASP:N	1:134:A:ASP:CA	1:134:A:ASP:C	1:135:A:ALA:N	2	1.81
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	15	1.81
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	3	1.81
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	3	1.8
(1,887)	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	1:78:D:VAL:N	5	1.8
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	1	1.8
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	9	1.8
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	16	1.8

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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	9	1.8
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	5	1.8
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	10	1.8
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	12	1.8
(1,801)	1:33:D:GLN:N	1:33:D:GLN:CA	1:33:D:GLN:C	1:34:D:LYS:N	1	1.79
(1,784)	1:22:D:SER:C	1:23:D:PHE:N	1:23:D:PHE:CA	1:23:D:PHE:C	18	1.79
(1,567)	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	1:43:C:ASP:N	19	1.79
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	8	1.79
(1,259)	1:11:B:PHE:N	1:11:B:PHE:CA	1:11:B:PHE:C	1:12:B:GLN:N	18	1.79
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	1	1.79
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	14	1.79
(1,709)	1:115:C:THR:N	1:115:C:THR:CA	1:115:C:THR:C	1:116:C:SER:N	18	1.78
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	13	1.78
(1,526)	1:18:C:THR:C	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	5	1.78
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	20	1.78
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	11	1.78
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	15	1.78
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	6	1.78
(1,254)	1:8:B:GLU:C	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	7	1.78
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	6	1.78
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	15	1.77
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	16	1.77
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	16	1.77
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1	1.77
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	13	1.77
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	16	1.77
(1,139)	1:81:A:GLY:N	1:81:A:GLY:CA	1:81:A:GLY:C	1:82:A:GLY:N	13	1.77
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	9	1.77
(1,52)	1:36:A:TRP:C	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	6	1.77
(1,474)	1:124:B:PRO:C	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	7	1.76
(1,385)	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	1:78:B:VAL:N	12	1.76
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	17	1.76
(1,310)	1:39:B:GLU:C	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1	1.76
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	17	1.76
(1,913)	1:90:D:GLU:N	1:90:D:GLU:CA	1:90:D:GLU:C	1:91:D:GLY:N	18	1.75
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	15	1.75
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	13	1.75
(1,556)	1:35:C:ASP:C	1:36:C:TRP:N	1:36:C:TRP:CA	1:36:C:TRP:C	9	1.75
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1	1.75
(1,305)	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1:37:B:GLN:N	11	1.75
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	19	1.75
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	13	1.75
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	5	1.74
(1,686)	1:101:C:TYR:C	1:102:C:CYS:N	1:102:C:CYS:CA	1:102:C:CYS:C	8	1.74
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	13	1.74
(1,366)	1:67:B:SER:C	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	18	1.74
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	7	1.74
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	5	1.74
(1,38)	1:29:A:PRO:C	1:30:A:HIS:N	1:30:A:HIS:CA	1:30:A:HIS:C	16	1.74
(1,8)	1:12:A:GLN:C	1:13:A:ILE:N	1:13:A:ILE:CA	1:13:A:ILE:C	7	1.74
(1,1012)	1:143:D:GLN:C	1:144:D:GLN:N	1:144:D:GLN:CA	1:144:D:GLN:C	12	1.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	6	1.73
(1,833)	1:50:D:GLN:N	1:50:D:GLN:CA	1:50:D:GLN:C	1:51:D:LEU:N	17	1.73
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	8	1.73
(1,400)	1:84:B:PHE:C	1:85:B:SER:N	1:85:B:SER:CA	1:85:B:SER:C	17	1.73
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	3	1.73
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	9	1.73
(1,96)	1:59:A:VAL:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	13	1.73
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	19	1.72
(1,579)	1:48:C:SER:N	1:48:C:SER:CA	1:48:C:SER:C	1:49:C:SER:N	18	1.72
(1,508)	1:9:C:MET:C	1:10:C:THR:N	1:10:C:THR:CA	1:10:C:THR:C	3	1.72
(1,384)	1:76:B:CYS:C	1:77:B:GLU:N	1:77:B:GLU:CA	1:77:B:GLU:C	1	1.72
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	19	1.72
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	14	1.72
(1,267)	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	1:16:B:ILE:N	18	1.72
(1,163)	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	1:94:A:MET:N	13	1.72
(1,148)	1:85:A:SER:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	14	1.72
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	11	1.71
(1,537)	1:24:C:GLU:N	1:24:C:GLU:CA	1:24:C:GLU:C	1:25:C:ALA:N	5	1.71
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	9	1.71
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	5	1.71
(1,92)	1:57:A:GLU:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	6	1.71
(1,92)	1:57:A:GLU:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	8	1.71
(1,59)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	5	1.71
(1,13)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ILE:N	12	1.71
(1,821)	1:44:D:LEU:N	1:44:D:LEU:CA	1:44:D:LEU:C	1:45:D:ASP:N	10	1.7
(1,812)	1:39:D:GLU:C	1:40:D:VAL:N	1:40:D:VAL:CA	1:40:D:VAL:C	5	1.7
(1,644)	1:80:C:GLN:C	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	4	1.7
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	10	1.7
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	20	1.7
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	6	1.7
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	17	1.7
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	20	1.7
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	3	1.69
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	7	1.69
(1,819)	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	1:44:D:LEU:N	19	1.69
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1	1.69
(1,755)	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	1:141:C:LEU:N	14	1.69
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	9	1.69
(1,510)	1:10:C:THR:C	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	6	1.69
(1,507)	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	1:10:C:THR:N	4	1.69
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	19	1.69
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	8	1.69
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	11	1.69
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	18	1.69
(1,79)	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	1:52:A:ALA:N	16	1.69
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	8	1.69
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	18	1.69
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	9	1.68
(1,660)	1:88:C:GLY:C	1:89:C:ILE:N	1:89:C:ILE:CA	1:89:C:ILE:C	17	1.68
(1,610)	1:63:C:THR:C	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	17	1.68
(1,478)	1:126:B:LEU:C	1:127:B:ASN:N	1:127:B:ASN:CA	1:127:B:ASN:C	5	1.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	20	1.68
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	3	1.68
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	12	1.68
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	8	1.68
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	14	1.67
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	15	1.67
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	10	1.67
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	20	1.67
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	9	1.67
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	10	1.67
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	14	1.66
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	20	1.66
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	20	1.66
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	16	1.66
(1,568)	1:42:C:LEU:C	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	4	1.66
(1,511)	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	1:12:C:GLN:N	19	1.66
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	2	1.66
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	17	1.66
(1,148)	1:85:A:SER:C	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	20	1.66
(1,97)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:ARG:N	13	1.66
(1,86)	1:54:A:ASP:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	4	1.66
(1,908)	1:87:D:ALA:C	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	4	1.65
(1,747)	1:136:C:LEU:N	1:136:C:LEU:CA	1:136:C:LEU:C	1:137:C:PHE:N	16	1.65
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	13	1.65
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	18	1.65
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1	1.65
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	6	1.65
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	4	1.65
(1,133)	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	1:79:A:GLN:N	13	1.65
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	13	1.65
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	9	1.64
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	8	1.64
(1,415)	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	1:93:B:GLN:N	18	1.64
(1,76)	1:49:A:SER:C	1:50:A:GLN:N	1:50:A:GLN:CA	1:50:A:GLN:C	15	1.64
(1,826)	1:46:D:THR:C	1:47:D:ALA:N	1:47:D:ALA:CA	1:47:D:ALA:C	7	1.63
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	14	1.63
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	17	1.63
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	1	1.63
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	2	1.62
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	12	1.62
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	8	1.62
(1,362)	1:65:B:THR:C	1:66:B:ALA:N	1:66:B:ALA:CA	1:66:B:ALA:C	20	1.62
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	17	1.62
(1,273)	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	1:19:B:LYS:N	14	1.62
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	18	1.62
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	14	1.62
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	16	1.61
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	3	1.61
(1,349)	1:59:B:VAL:N	1:59:B:VAL:CA	1:59:B:VAL:C	1:60:B:LEU:N	16	1.61
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	10	1.61
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	19	1.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	8	1.61
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	9	1.61
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	9	1.61
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	15	1.61
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	7	1.6
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	2	1.6
(1,894)	1:80:D:GLN:C	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	3	1.6
(1,887)	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	1:78:D:VAL:N	17	1.6
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	15	1.6
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	2	1.6
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	9	1.6
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	1	1.6
(1,158)	1:90:A:GLU:C	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	7	1.6
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	16	1.6
(1,108)	1:65:A:THR:C	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	8	1.6
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	9	1.6
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	5	1.59
(1,848)	1:57:D:GLU:C	1:58:D:VAL:N	1:58:D:VAL:CA	1:58:D:VAL:C	8	1.59
(1,810)	1:38:D:PRO:C	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	4	1.59
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	10	1.59
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	18	1.59
(1,655)	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	1:87:C:ALA:N	1	1.59
(1,579)	1:48:C:SER:N	1:48:C:SER:CA	1:48:C:SER:C	1:49:C:SER:N	11	1.59
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	8	1.59
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	18	1.59
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	12	1.59
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	16	1.59
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	17	1.58
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	11	1.58
(1,727)	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1:126:C:LEU:N	12	1.58
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	1	1.58
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	19	1.58
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	17	1.58
(1,37)	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1:29:A:PRO:N	5	1.58
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	8	1.58
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	4	1.57
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	5	1.57
(1,905)	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	1:87:D:ALA:N	4	1.57
(1,901)	1:84:D:PHE:N	1:84:D:PHE:CA	1:84:D:PHE:C	1:85:D:SER:N	16	1.57
(1,835)	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	1:52:D:ALA:N	16	1.57
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	6	1.57
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	15	1.57
(1,430)	1:99:B:GLY:C	1:100:B:ALA:N	1:100:B:ALA:CA	1:100:B:ALA:C	16	1.57
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	15	1.57
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	10	1.57
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	12	1.57
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	20	1.57
(1,773)	1:17:D:TYR:N	1:17:D:TYR:CA	1:17:D:TYR:C	1:18:D:THR:N	8	1.56
(1,383)	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	1:77:B:GLU:N	1	1.56
(1,136)	1:79:A:GLN:C	1:80:A:GLN:N	1:80:A:GLN:CA	1:80:A:GLN:C	2	1.56
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	3	1.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,1006)	1:140:D:TYR:C	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	10	1.55
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	7	1.55
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	3	1.55
(1,787)	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	1:25:D:ALA:N	13	1.55
(1,763)	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	1:13:D:ILE:N	4	1.55
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	2	1.55
(1,570)	1:43:C:ASP:C	1:44:C:LEU:N	1:44:C:LEU:CA	1:44:C:LEU:C	18	1.55
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	4	1.55
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	10	1.55
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	13	1.55
(1,251)	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	1:142:A:GLN:N	1	1.55
(1,230)	1:130:A:PRO:C	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	5	1.55
(1,145)	1:84:A:PHE:N	1:84:A:PHE:CA	1:84:A:PHE:C	1:85:A:SER:N	3	1.55
(1,90)	1:56:A:TYR:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	13	1.55
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	6	1.55
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	18	1.54
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	10	1.54
(1,404)	1:86:B:ILE:C	1:87:B:ALA:N	1:87:B:ALA:CA	1:87:B:ALA:C	8	1.54
(1,324)	1:46:B:THR:C	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	5	1.54
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	10	1.54
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	1	1.54
(1,171)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:LEU:N	16	1.54
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	16	1.54
(1,152)	1:87:A:ALA:C	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	5	1.54
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	7	1.54
(1,37)	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1:29:A:PRO:N	12	1.54
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	10	1.53
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	10	1.53
(1,748)	1:136:C:LEU:C	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	15	1.53
(1,639)	1:78:C:VAL:N	1:78:C:VAL:CA	1:78:C:VAL:C	1:79:C:GLN:N	19	1.53
(1,489)	1:133:B:PHE:N	1:133:B:PHE:CA	1:133:B:PHE:C	1:134:B:ASP:N	9	1.53
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	2	1.53
(1,372)	1:70:B:GLU:C	1:71:B:GLU:N	1:71:B:GLU:CA	1:71:B:GLU:C	7	1.53
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	20	1.53
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	15	1.53
(1,252)	1:141:A:LEU:C	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	13	1.53
(1,92)	1:57:A:GLU:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	16	1.53
(1,80)	1:51:A:LEU:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	6	1.53
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	5	1.52
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	13	1.52
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	12	1.52
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	3	1.52
(1,17)	1:17:A:TYR:N	1:17:A:TYR:CA	1:17:A:TYR:C	1:18:A:THR:N	13	1.52
(1,911)	1:89:D:ILE:N	1:89:D:ILE:CA	1:89:D:ILE:C	1:90:D:GLU:N	6	1.51
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	5	1.51
(1,643)	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	1:81:C:GLY:N	17	1.51
(1,546)	1:30:C:HIS:C	1:31:C:VAL:N	1:31:C:VAL:CA	1:31:C:VAL:C	10	1.51
(1,523)	1:17:C:TYR:N	1:17:C:TYR:CA	1:17:C:TYR:C	1:18:C:THR:N	2	1.51
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	13	1.51
(1,303)	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	1:36:B:TRP:N	18	1.51
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	10	1.51

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	17	1.51
(1,53)	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1:38:A:PRO:N	4	1.51
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	3	1.51
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	16	1.5
(1,314)	1:41:B:LYS:C	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	17	1.5
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	7	1.5
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	7	1.5
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	16	1.5
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	19	1.49
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	4	1.49
(1,835)	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	1:52:D:ALA:N	18	1.49
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	1	1.49
(1,731)	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	1:128:C:LEU:N	1	1.49
(1,623)	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1:71:C:GLU:N	2	1.49
(1,577)	1:47:C:ALA:N	1:47:C:ALA:CA	1:47:C:ALA:C	1:48:C:SER:N	11	1.49
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	1	1.49
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	11	1.49
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	2	1.49
(1,1007)	1:141:D:LEU:N	1:141:D:LEU:CA	1:141:D:LEU:C	1:142:D:GLN:N	15	1.48
(1,645)	1:81:C:GLY:N	1:81:C:GLY:CA	1:81:C:GLY:C	1:82:C:GLY:N	10	1.48
(1,344)	1:56:B:TYR:C	1:57:B:GLU:N	1:57:B:GLU:CA	1:57:B:GLU:C	10	1.48
(1,300)	1:33:B:GLN:C	1:34:B:LYS:N	1:34:B:LYS:CA	1:34:B:LYS:C	7	1.48
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	1	1.48
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	8	1.48
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	7	1.48
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	14	1.47
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	17	1.47
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	6	1.47
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	17	1.47
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	11	1.47
(1,407)	1:88:B:GLY:N	1:88:B:GLY:CA	1:88:B:GLY:C	1:89:B:ILE:N	9	1.47
(1,173)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:GLY:N	2	1.47
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	17	1.47
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	17	1.47
(1,889)	1:78:D:VAL:N	1:78:D:VAL:CA	1:78:D:VAL:C	1:79:D:GLN:N	4	1.46
(1,647)	1:82:C:GLY:N	1:82:C:GLY:CA	1:82:C:GLY:C	1:83:C:ILE:N	19	1.46
(1,538)	1:24:C:GLU:C	1:25:C:ALA:N	1:25:C:ALA:CA	1:25:C:ALA:C	8	1.46
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	16	1.46
(1,402)	1:85:B:SER:C	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	10	1.46
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	9	1.46
(1,343)	1:56:B:TYR:N	1:56:B:TYR:CA	1:56:B:TYR:C	1:57:B:GLU:N	14	1.46
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	12	1.46
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	7	1.46
(1,287)	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	1:26:B:PRO:N	20	1.46
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	11	1.46
(1,131)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:VAL:N	12	1.46
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	17	1.46
(1,986)	1:130:D:PRO:C	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	15	1.45
(1,985)	1:129:D:ALA:N	1:129:D:ALA:CA	1:129:D:ALA:C	1:130:D:PRO:N	12	1.45
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	8	1.45
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	18	1.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	3	1.45
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	19	1.45
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	5	1.45
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	18	1.45
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	20	1.45
(1,120)	1:71:A:GLU:C	1:72:A:THR:N	1:72:A:THR:CA	1:72:A:THR:C	1	1.45
(1,98)	1:60:A:LEU:C	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	20	1.45
(1,96)	1:59:A:VAL:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	2	1.45
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	16	1.45
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	4	1.45
(1,906)	1:86:D:ILE:C	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	19	1.44
(1,884)	1:75:D:LEU:C	1:76:D:CYS:N	1:76:D:CYS:CA	1:76:D:CYS:C	8	1.44
(1,880)	1:73:D:ALA:C	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	13	1.44
(1,868)	1:67:D:SER:C	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	12	1.44
(1,855)	1:61:D:ARG:N	1:61:D:ARG:CA	1:61:D:ARG:C	1:62:D:VAL:N	12	1.44
(1,824)	1:45:D:ASP:C	1:46:D:THR:N	1:46:D:THR:CA	1:46:D:THR:C	11	1.44
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	4	1.44
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	18	1.44
(1,564)	1:40:C:VAL:C	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	17	1.44
(1,552)	1:33:C:GLN:C	1:34:C:LYS:N	1:34:C:LYS:CA	1:34:C:LYS:C	20	1.44
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	12	1.44
(1,381)	1:75:B:LEU:N	1:75:B:LEU:CA	1:75:B:LEU:C	1:76:B:CYS:N	14	1.44
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	12	1.44
(1,325)	1:47:B:ALA:N	1:47:B:ALA:CA	1:47:B:ALA:C	1:48:B:SER:N	16	1.44
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	3	1.44
(1,49)	1:35:A:ASP:N	1:35:A:ASP:CA	1:35:A:ASP:C	1:36:A:TRP:N	15	1.44
(1,974)	1:122:D:THR:C	1:123:D:PHE:N	1:123:D:PHE:CA	1:123:D:PHE:C	3	1.43
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	11	1.43
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	10	1.43
(1,736)	1:130:C:PRO:C	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	5	1.43
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	3	1.43
(1,412)	1:90:B:GLU:C	1:91:B:GLY:N	1:91:B:GLY:CA	1:91:B:GLY:C	12	1.43
(1,152)	1:87:A:ALA:C	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	2	1.43
(1,1)	1:9:A:MET:N	1:9:A:MET:CA	1:9:A:MET:C	1:10:A:THR:N	4	1.43
(1,835)	1:51:D:LEU:N	1:51:D:LEU:CA	1:51:D:LEU:C	1:52:D:ALA:N	3	1.42
(1,788)	1:24:D:GLU:C	1:25:D:ALA:N	1:25:D:ALA:CA	1:25:D:ALA:C	8	1.42
(1,741)	1:133:C:PHE:N	1:133:C:PHE:CA	1:133:C:PHE:C	1:134:C:ASP:N	18	1.42
(1,636)	1:76:C:CYS:C	1:77:C:GLU:N	1:77:C:GLU:CA	1:77:C:GLU:C	18	1.42
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	11	1.42
(1,315)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:ASP:N	12	1.42
(1,302)	1:34:B:LYS:C	1:35:B:ASP:N	1:35:B:ASP:CA	1:35:B:ASP:C	15	1.42
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	13	1.42
(1,130)	1:76:A:CYS:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	2	1.42
(1,116)	1:69:A:GLY:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	3	1.42
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	7	1.42
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	20	1.41
(1,412)	1:90:B:GLU:C	1:91:B:GLY:N	1:91:B:GLY:CA	1:91:B:GLY:C	2	1.41
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	14	1.41
(1,173)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:GLY:N	16	1.41
(1,127)	1:75:A:LEU:N	1:75:A:LEU:CA	1:75:A:LEU:C	1:76:A:CYS:N	18	1.41
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	1	1.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,830)	1:48:D:SER:C	1:49:D:SER:N	1:49:D:SER:CA	1:49:D:SER:C	7	1.4
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	16	1.4
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	5	1.4
(1,393)	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1:82:B:GLY:N	16	1.4
(1,326)	1:47:B:ALA:C	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	20	1.4
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	10	1.4
(1,65)	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	1:45:A:ASP:N	9	1.4
(1,850)	1:58:D:VAL:C	1:59:D:VAL:N	1:59:D:VAL:CA	1:59:D:VAL:C	10	1.39
(1,810)	1:38:D:PRO:C	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	7	1.39
(1,788)	1:24:D:GLU:C	1:25:D:ALA:N	1:25:D:ALA:CA	1:25:D:ALA:C	1	1.39
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	20	1.39
(1,622)	1:69:C:GLY:C	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	4	1.39
(1,572)	1:44:C:LEU:C	1:45:C:ASP:N	1:45:C:ASP:CA	1:45:C:ASP:C	12	1.39
(1,396)	1:82:B:GLY:C	1:83:B:ILE:N	1:83:B:ILE:CA	1:83:B:ILE:C	10	1.39
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	15	1.39
(1,317)	1:43:B:ASP:N	1:43:B:ASP:CA	1:43:B:ASP:C	1:44:B:LEU:N	6	1.39
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	12	1.39
(1,85)	1:54:A:ASP:N	1:54:A:ASP:CA	1:54:A:ASP:C	1:55:A:VAL:N	9	1.39
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	13	1.39
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	8	1.38
(1,651)	1:84:C:PHE:N	1:84:C:PHE:CA	1:84:C:PHE:C	1:85:C:SER:N	20	1.38
(1,593)	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	1:56:C:TYR:N	8	1.38
(1,419)	1:94:B:MET:N	1:94:B:MET:CA	1:94:B:MET:C	1:95:B:ALA:N	11	1.38
(1,311)	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	1:41:B:LYS:N	9	1.38
(1,272)	1:17:B:TYR:C	1:18:B:THR:N	1:18:B:THR:CA	1:18:B:THR:C	11	1.38
(1,153)	1:88:A:GLY:N	1:88:A:GLY:CA	1:88:A:GLY:C	1:89:A:ILE:N	20	1.38
(1,140)	1:81:A:GLY:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	15	1.38
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	14	1.38
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	19	1.38
(1,24)	1:20:A:ASP:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	7	1.38
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	7	1.37
(1,655)	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	1:87:C:ALA:N	3	1.37
(1,429)	1:99:B:GLY:N	1:99:B:GLY:CA	1:99:B:GLY:C	1:100:B:ALA:N	12	1.37
(1,328)	1:48:B:SER:C	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1	1.37
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	2	1.37
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	5	1.37
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	11	1.37
(1,36)	1:27:A:ASN:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	18	1.37
(1,895)	1:81:D:GLY:N	1:81:D:GLY:CA	1:81:D:GLY:C	1:82:D:GLY:N	1	1.36
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	5	1.36
(1,527)	1:19:C:LYS:N	1:19:C:LYS:CA	1:19:C:LYS:C	1:20:C:ASP:N	2	1.36
(1,310)	1:39:B:GLU:C	1:40:B:VAL:N	1:40:B:VAL:CA	1:40:B:VAL:C	15	1.36
(1,109)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:SER:N	18	1.36
(1,108)	1:65:A:THR:C	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	18	1.36
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	16	1.36
(1,69)	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1:47:A:ALA:N	13	1.36
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	20	1.36
(1,4)	1:10:A:THR:C	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	4	1.36
(1,319)	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	1:45:B:ASP:N	2	1.35
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	18	1.35
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	16	1.35

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:VAL:N	18	1.35
(1,906)	1:86:D:ILE:C	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1	1.34
(1,905)	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	1:87:D:ALA:N	2	1.34
(1,864)	1:65:D:THR:C	1:66:D:ALA:N	1:66:D:ALA:CA	1:66:D:ALA:C	20	1.34
(1,766)	1:13:D:ILE:C	1:14:D:GLN:N	1:14:D:GLN:CA	1:14:D:GLN:C	6	1.34
(1,510)	1:10:C:THR:C	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	10	1.34
(1,284)	1:23:B:PHE:C	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	17	1.34
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	6	1.34
(1,748)	1:136:C:LEU:C	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	3	1.33
(1,709)	1:115:C:THR:N	1:115:C:THR:CA	1:115:C:THR:C	1:116:C:SER:N	15	1.33
(1,643)	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	1:81:C:GLY:N	18	1.33
(1,392)	1:80:B:GLN:C	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	11	1.33
(1,305)	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1:37:B:GLN:N	3	1.33
(1,252)	1:141:A:LEU:C	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	15	1.33
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	15	1.33
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	2	1.33
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	6	1.33
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	9	1.32
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	16	1.32
(1,659)	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	1:89:C:ILE:N	7	1.32
(1,655)	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	1:87:C:ALA:N	14	1.32
(1,640)	1:78:C:VAL:C	1:79:C:GLN:N	1:79:C:GLN:CA	1:79:C:GLN:C	13	1.32
(1,609)	1:63:C:THR:N	1:63:C:THR:CA	1:63:C:THR:C	1:64:C:VAL:N	12	1.32
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	4	1.32
(1,559)	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	1:38:C:PRO:N	4	1.32
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	6	1.32
(1,476)	1:125:B:GLN:C	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	19	1.32
(1,154)	1:88:A:GLY:C	1:89:A:ILE:N	1:89:A:ILE:CA	1:89:A:ILE:C	10	1.32
(1,95)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:LEU:N	20	1.32
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	15	1.32
(1,909)	1:88:D:GLY:N	1:88:D:GLY:CA	1:88:D:GLY:C	1:89:D:ILE:N	2	1.31
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	20	1.31
(1,889)	1:78:D:VAL:N	1:78:D:VAL:CA	1:78:D:VAL:C	1:79:D:GLN:N	18	1.31
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	6	1.31
(1,253)	1:142:A:GLN:N	1:142:A:GLN:CA	1:142:A:GLN:C	1:143:A:GLN:N	9	1.31
(1,231)	1:131:A:VAL:N	1:131:A:VAL:CA	1:131:A:VAL:C	1:132:A:ASN:N	16	1.31
(1,109)	1:66:A:ALA:N	1:66:A:ALA:CA	1:66:A:ALA:C	1:67:A:SER:N	6	1.31
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	13	1.31
(1,102)	1:62:A:VAL:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	16	1.31
(1,71)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:SER:N	14	1.31
(1,987)	1:131:D:VAL:N	1:131:D:VAL:CA	1:131:D:VAL:C	1:132:D:ASN:N	18	1.3
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	13	1.3
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	18	1.3
(1,623)	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1:71:C:GLU:N	12	1.3
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	3	1.3
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	4	1.3
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	1	1.3
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	9	1.3
(1,162)	1:92:A:THR:C	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	12	1.3
(1,142)	1:82:A:GLY:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	12	1.3
(1,106)	1:64:A:VAL:C	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	5	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,88)	1:55:A:VAL:C	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	9	1.3
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	1	1.3
(1,1011)	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	1:144:D:GLN:N	1	1.29
(1,861)	1:64:D:VAL:N	1:64:D:VAL:CA	1:64:D:VAL:C	1:65:D:THR:N	5	1.29
(1,839)	1:53:D:ASP:N	1:53:D:ASP:CA	1:53:D:ASP:C	1:54:D:ASP:N	6	1.29
(1,818)	1:42:D:LEU:C	1:43:D:ASP:N	1:43:D:ASP:CA	1:43:D:ASP:C	3	1.29
(1,58)	1:40:A:VAL:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	2	1.29
(1,36)	1:27:A:ASN:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	11	1.29
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	3	1.28
(1,880)	1:73:D:ALA:C	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	8	1.28
(1,817)	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	1:43:D:ASP:N	8	1.28
(1,815)	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	1:42:D:LEU:N	12	1.28
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	2	1.28
(1,574)	1:45:C:ASP:C	1:46:C:THR:N	1:46:C:THR:CA	1:46:C:THR:C	16	1.28
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	17	1.28
(1,408)	1:88:B:GLY:C	1:89:B:ILE:N	1:89:B:ILE:CA	1:89:B:ILE:C	6	1.28
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	13	1.28
(1,361)	1:65:B:THR:N	1:65:B:THR:CA	1:65:B:THR:C	1:66:B:ALA:N	11	1.28
(1,250)	1:140:A:TYR:C	1:141:A:LEU:N	1:141:A:LEU:CA	1:141:A:LEU:C	2	1.28
(1,30)	1:23:A:PHE:C	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	12	1.28
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	6	1.27
(1,790)	1:26:D:PRO:C	1:27:D:ASN:N	1:27:D:ASN:CA	1:27:D:ASN:C	13	1.27
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	16	1.27
(1,741)	1:133:C:PHE:N	1:133:C:PHE:CA	1:133:C:PHE:C	1:134:C:ASP:N	19	1.27
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	19	1.27
(1,476)	1:125:B:GLN:C	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	10	1.27
(1,355)	1:62:B:VAL:N	1:62:B:VAL:CA	1:62:B:VAL:C	1:63:B:THR:N	14	1.27
(1,332)	1:50:B:GLN:C	1:51:B:LEU:N	1:51:B:LEU:CA	1:51:B:LEU:C	2	1.27
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	2	1.27
(1,292)	1:29:B:PRO:C	1:30:B:HIS:N	1:30:B:HIS:CA	1:30:B:HIS:C	14	1.27
(1,217)	1:122:A:THR:N	1:122:A:THR:CA	1:122:A:THR:C	1:123:A:PHE:N	20	1.27
(1,89)	1:56:A:TYR:N	1:56:A:TYR:CA	1:56:A:TYR:C	1:57:A:GLU:N	2	1.27
(1,14)	1:15:A:ARG:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	20	1.27
(1,985)	1:129:D:ALA:N	1:129:D:ALA:CA	1:129:D:ALA:C	1:130:D:PRO:N	14	1.26
(1,982)	1:127:D:ASN:C	1:128:D:LEU:N	1:128:D:LEU:CA	1:128:D:LEU:C	16	1.26
(1,898)	1:82:D:GLY:C	1:83:D:ILE:N	1:83:D:ILE:CA	1:83:D:ILE:C	3	1.26
(1,861)	1:64:D:VAL:N	1:64:D:VAL:CA	1:64:D:VAL:C	1:65:D:THR:N	20	1.26
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	1	1.26
(1,754)	1:139:C:ASN:C	1:140:C:TYR:N	1:140:C:TYR:CA	1:140:C:TYR:C	14	1.26
(1,500)	1:138:B:MET:C	1:139:B:ASN:N	1:139:B:ASN:CA	1:139:B:ASN:C	15	1.26
(1,53)	1:37:A:GLN:N	1:37:A:GLN:CA	1:37:A:GLN:C	1:38:A:PRO:N	12	1.26
(1,901)	1:84:D:PHE:N	1:84:D:PHE:CA	1:84:D:PHE:C	1:85:D:SER:N	12	1.25
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	8	1.25
(1,559)	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	1:38:C:PRO:N	3	1.25
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	3	1.25
(1,506)	1:8:C:GLU:C	1:9:C:MET:N	1:9:C:MET:CA	1:9:C:MET:C	15	1.25
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	9	1.24
(1,382)	1:75:B:LEU:C	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	2	1.24
(1,321)	1:45:B:ASP:N	1:45:B:ASP:CA	1:45:B:ASP:C	1:46:B:THR:N	3	1.24
(1,110)	1:66:A:ALA:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	11	1.24
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	14	1.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,563)	1:40:C:VAL:N	1:40:C:VAL:CA	1:40:C:VAL:C	1:41:C:LYS:N	10	1.23
(1,505)	1:141:B:LEU:N	1:141:B:LEU:CA	1:141:B:LEU:C	1:142:B:GLN:N	9	1.23
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	8	1.23
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	14	1.23
(1,102)	1:62:A:VAL:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	18	1.23
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	15	1.22
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	18	1.22
(1,678)	1:97:C:CYS:C	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	8	1.22
(1,623)	1:70:C:GLU:N	1:70:C:GLU:CA	1:70:C:GLU:C	1:71:C:GLU:N	17	1.22
(1,510)	1:10:C:THR:C	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	4	1.22
(1,383)	1:76:B:CYS:N	1:76:B:CYS:CA	1:76:B:CYS:C	1:77:B:GLU:N	6	1.22
(1,129)	1:76:A:CYS:N	1:76:A:CYS:CA	1:76:A:CYS:C	1:77:A:GLU:N	2	1.22
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	15	1.22
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	6	1.22
(1,72)	1:47:A:ALA:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	8	1.22
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	16	1.21
(1,678)	1:97:C:CYS:C	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	18	1.21
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	2	1.21
(1,602)	1:59:C:VAL:C	1:60:C:LEU:N	1:60:C:LEU:CA	1:60:C:LEU:C	13	1.21
(1,550)	1:32:C:PHE:C	1:33:C:GLN:N	1:33:C:GLN:CA	1:33:C:GLN:C	13	1.21
(1,550)	1:32:C:PHE:C	1:33:C:GLN:N	1:33:C:GLN:CA	1:33:C:GLN:C	15	1.21
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	12	1.21
(1,286)	1:24:B:GLU:C	1:25:B:ALA:N	1:25:B:ALA:CA	1:25:B:ALA:C	16	1.21
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	15	1.21
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	10	1.21
(1,111)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:LEU:N	6	1.21
(1,96)	1:59:A:VAL:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	20	1.21
(1,869)	1:68:D:LEU:N	1:68:D:LEU:CA	1:68:D:LEU:C	1:69:D:GLY:N	12	1.2
(1,831)	1:49:D:SER:N	1:49:D:SER:CA	1:49:D:SER:C	1:50:D:GLN:N	4	1.2
(1,802)	1:33:D:GLN:C	1:34:D:LYS:N	1:34:D:LYS:CA	1:34:D:LYS:C	9	1.2
(1,726)	1:124:C:PRO:C	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	11	1.2
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	10	1.2
(1,643)	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	1:81:C:GLY:N	14	1.2
(1,580)	1:48:C:SER:C	1:49:C:SER:N	1:49:C:SER:CA	1:49:C:SER:C	1	1.2
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	15	1.2
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	12	1.2
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	4	1.2
(1,904)	1:85:D:SER:C	1:86:D:ILE:N	1:86:D:ILE:CA	1:86:D:ILE:C	10	1.19
(1,897)	1:82:D:GLY:N	1:82:D:GLY:CA	1:82:D:GLY:C	1:83:D:ILE:N	10	1.19
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	7	1.19
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	14	1.19
(1,579)	1:48:C:SER:N	1:48:C:SER:CA	1:48:C:SER:C	1:49:C:SER:N	10	1.19
(1,565)	1:41:C:LYS:N	1:41:C:LYS:CA	1:41:C:LYS:C	1:42:C:LEU:N	15	1.19
(1,428)	1:98:B:LEU:C	1:99:B:GLY:N	1:99:B:GLY:CA	1:99:B:GLY:C	6	1.19
(1,294)	1:30:B:HIS:C	1:31:B:VAL:N	1:31:B:VAL:CA	1:31:B:VAL:C	10	1.19
(1,141)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:ILE:N	5	1.19
(1,73)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	20	1.19
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	20	1.18
(1,753)	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1:140:C:TYR:N	7	1.18
(1,654)	1:85:C:SER:C	1:86:C:ILE:N	1:86:C:ILE:CA	1:86:C:ILE:C	10	1.18
(1,429)	1:99:B:GLY:N	1:99:B:GLY:CA	1:99:B:GLY:C	1:100:B:ALA:N	8	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,386)	1:77:B:GLU:C	1:78:B:VAL:N	1:78:B:VAL:CA	1:78:B:VAL:C	17	1.18
(1,285)	1:24:B:GLU:N	1:24:B:GLU:CA	1:24:B:GLU:C	1:25:B:ALA:N	1	1.18
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	14	1.18
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	6	1.18
(1,95)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:LEU:N	13	1.18
(1,94)	1:58:A:VAL:C	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	6	1.18
(1,40)	1:30:A:HIS:C	1:31:A:VAL:N	1:31:A:VAL:CA	1:31:A:VAL:C	9	1.18
(1,1010)	1:142:D:GLN:C	1:143:D:GLN:N	1:143:D:GLN:CA	1:143:D:GLN:C	15	1.17
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	13	1.17
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	8	1.17
(1,796)	1:30:D:HIS:C	1:31:D:VAL:N	1:31:D:VAL:CA	1:31:D:VAL:C	20	1.17
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	18	1.17
(1,617)	1:67:C:SER:N	1:67:C:SER:CA	1:67:C:SER:C	1:68:C:LEU:N	4	1.17
(1,566)	1:41:C:LYS:C	1:42:C:LEU:N	1:42:C:LEU:CA	1:42:C:LEU:C	15	1.17
(1,555)	1:35:C:ASP:N	1:35:C:ASP:CA	1:35:C:ASP:C	1:36:C:TRP:N	10	1.17
(1,414)	1:91:B:GLY:C	1:92:B:THR:N	1:92:B:THR:CA	1:92:B:THR:C	4	1.17
(1,161)	1:92:A:THR:N	1:92:A:THR:CA	1:92:A:THR:C	1:93:A:GLN:N	11	1.17
(1,135)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:GLN:N	16	1.17
(1,70)	1:46:A:THR:C	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	6	1.17
(1,46)	1:33:A:GLN:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	2	1.17
(1,11)	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	1:15:A:ARG:N	13	1.17
(1,862)	1:64:D:VAL:C	1:65:D:THR:N	1:65:D:THR:CA	1:65:D:THR:C	11	1.16
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	5	1.16
(1,665)	1:91:C:GLY:N	1:91:C:GLY:CA	1:91:C:GLY:C	1:92:C:THR:N	20	1.16
(1,569)	1:43:C:ASP:N	1:43:C:ASP:CA	1:43:C:ASP:C	1:44:C:LEU:N	7	1.16
(1,544)	1:29:C:PRO:C	1:30:C:HIS:N	1:30:C:HIS:CA	1:30:C:HIS:C	6	1.16
(1,329)	1:49:B:SER:N	1:49:B:SER:CA	1:49:B:SER:C	1:50:B:GLN:N	16	1.16
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	9	1.16
(1,265)	1:14:B:GLN:N	1:14:B:GLN:CA	1:14:B:GLN:C	1:15:B:ARG:N	11	1.16
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	18	1.16
(1,159)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:THR:N	5	1.16
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	16	1.16
(1,27)	1:22:A:SER:N	1:22:A:SER:CA	1:22:A:SER:C	1:23:A:PHE:N	5	1.16
(1,2)	1:9:A:MET:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	2	1.16
(1,880)	1:73:D:ALA:C	1:74:D:PHE:N	1:74:D:PHE:CA	1:74:D:PHE:C	9	1.15
(1,855)	1:61:D:ARG:N	1:61:D:ARG:CA	1:61:D:ARG:C	1:62:D:VAL:N	5	1.15
(1,805)	1:35:D:ASP:N	1:35:D:ASP:CA	1:35:D:ASP:C	1:36:D:TRP:N	11	1.15
(1,757)	1:9:D:MET:N	1:9:D:MET:CA	1:9:D:MET:C	1:10:D:THR:N	1	1.15
(1,533)	1:22:C:SER:N	1:22:C:SER:CA	1:22:C:SER:C	1:23:C:PHE:N	8	1.15
(1,339)	1:54:B:ASP:N	1:54:B:ASP:CA	1:54:B:ASP:C	1:55:B:VAL:N	20	1.15
(1,283)	1:23:B:PHE:N	1:23:B:PHE:CA	1:23:B:PHE:C	1:24:B:GLU:N	20	1.15
(1,134)	1:78:A:VAL:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	4	1.15
(1,132)	1:77:A:GLU:C	1:78:A:VAL:N	1:78:A:VAL:CA	1:78:A:VAL:C	6	1.15
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	18	1.15
(1,68)	1:45:A:ASP:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	12	1.15
(1,974)	1:122:D:THR:C	1:123:D:PHE:N	1:123:D:PHE:CA	1:123:D:PHE:C	19	1.14
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	1	1.14
(1,679)	1:98:C:LEU:N	1:98:C:LEU:CA	1:98:C:LEU:C	1:99:C:GLY:N	3	1.14
(1,558)	1:36:C:TRP:C	1:37:C:GLN:N	1:37:C:GLN:CA	1:37:C:GLN:C	8	1.14
(1,419)	1:94:B:MET:N	1:94:B:MET:CA	1:94:B:MET:C	1:95:B:ALA:N	10	1.14
(1,390)	1:79:B:GLN:C	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	20	1.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,31)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:ALA:N	4	1.14
(1,890)	1:78:D:VAL:C	1:79:D:GLN:N	1:79:D:GLN:CA	1:79:D:GLN:C	7	1.13
(1,857)	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	1:63:D:THR:N	7	1.13
(1,816)	1:41:D:LYS:C	1:42:D:LEU:N	1:42:D:LEU:CA	1:42:D:LEU:C	10	1.13
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	12	1.13
(1,662)	1:89:C:ILE:C	1:90:C:GLU:N	1:90:C:GLU:CA	1:90:C:GLU:C	6	1.13
(1,592)	1:54:C:ASP:C	1:55:C:VAL:N	1:55:C:VAL:CA	1:55:C:VAL:C	2	1.13
(1,475)	1:125:B:GLN:N	1:125:B:GLN:CA	1:125:B:GLN:C	1:126:B:LEU:N	11	1.13
(1,390)	1:79:B:GLN:C	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	3	1.13
(1,99)	1:61:A:ARG:N	1:61:A:ARG:CA	1:61:A:ARG:C	1:62:A:VAL:N	17	1.13
(1,78)	1:50:A:GLN:C	1:51:A:LEU:N	1:51:A:LEU:CA	1:51:A:LEU:C	12	1.13
(1,907)	1:87:D:ALA:N	1:87:D:ALA:CA	1:87:D:ALA:C	1:88:D:GLY:N	13	1.12
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	1	1.12
(1,850)	1:58:D:VAL:C	1:59:D:VAL:N	1:59:D:VAL:CA	1:59:D:VAL:C	12	1.12
(1,758)	1:9:D:MET:C	1:10:D:THR:N	1:10:D:THR:CA	1:10:D:THR:C	4	1.12
(1,625)	1:71:C:GLU:N	1:71:C:GLU:CA	1:71:C:GLU:C	1:72:C:THR:N	14	1.12
(1,579)	1:48:C:SER:N	1:48:C:SER:CA	1:48:C:SER:C	1:49:C:SER:N	14	1.12
(1,485)	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	1:132:B:ASN:N	5	1.12
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	3	1.12
(1,477)	1:126:B:LEU:N	1:126:B:LEU:CA	1:126:B:LEU:C	1:127:B:ASN:N	16	1.12
(1,356)	1:62:B:VAL:C	1:63:B:THR:N	1:63:B:THR:CA	1:63:B:THR:C	4	1.12
(1,255)	1:9:B:MET:N	1:9:B:MET:CA	1:9:B:MET:C	1:10:B:THR:N	9	1.12
(1,157)	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	1:91:A:GLY:N	12	1.12
(1,64)	1:43:A:ASP:C	1:44:A:LEU:N	1:44:A:LEU:CA	1:44:A:LEU:C	8	1.12
(1,927)	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	1:98:D:LEU:N	18	1.11
(1,871)	1:69:D:GLY:N	1:69:D:GLY:CA	1:69:D:GLY:C	1:70:D:GLU:N	11	1.11
(1,681)	1:99:C:GLY:N	1:99:C:GLY:CA	1:99:C:GLY:C	1:100:C:ALA:N	2	1.11
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	1	1.11
(1,499)	1:138:B:MET:N	1:138:B:MET:CA	1:138:B:MET:C	1:139:B:ASN:N	1	1.11
(1,403)	1:86:B:ILE:N	1:86:B:ILE:CA	1:86:B:ILE:C	1:87:B:ALA:N	18	1.11
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	19	1.11
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	20	1.11
(1,117)	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1:71:A:GLU:N	5	1.11
(1,107)	1:65:A:THR:N	1:65:A:THR:CA	1:65:A:THR:C	1:66:A:ALA:N	14	1.11
(1,100)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	10	1.11
(1,96)	1:59:A:VAL:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	17	1.11
(1,892)	1:79:D:GLN:C	1:80:D:GLN:N	1:80:D:GLN:CA	1:80:D:GLN:C	14	1.1
(1,858)	1:62:D:VAL:C	1:63:D:THR:N	1:63:D:THR:CA	1:63:D:THR:C	6	1.1
(1,855)	1:61:D:ARG:N	1:61:D:ARG:CA	1:61:D:ARG:C	1:62:D:VAL:N	13	1.1
(1,855)	1:61:D:ARG:N	1:61:D:ARG:CA	1:61:D:ARG:C	1:62:D:VAL:N	17	1.1
(1,752)	1:138:C:MET:C	1:139:C:ASN:N	1:139:C:ASN:CA	1:139:C:ASN:C	1	1.1
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	2	1.1
(1,318)	1:43:B:ASP:C	1:44:B:LEU:N	1:44:B:LEU:CA	1:44:B:LEU:C	16	1.1
(1,261)	1:12:B:GLN:N	1:12:B:GLN:CA	1:12:B:GLN:C	1:13:B:ILE:N	12	1.1
(1,163)	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	1:94:A:MET:N	17	1.1
(1,114)	1:68:A:LEU:C	1:69:A:GLY:N	1:69:A:GLY:CA	1:69:A:GLY:C	9	1.1
(1,28)	1:22:A:SER:C	1:23:A:PHE:N	1:23:A:PHE:CA	1:23:A:PHE:C	5	1.1
(1,21)	1:19:A:LYS:N	1:19:A:LYS:CA	1:19:A:LYS:C	1:20:A:ASP:N	10	1.1
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	1	1.09
(1,634)	1:75:C:LEU:C	1:76:C:CYS:N	1:76:C:CYS:CA	1:76:C:CYS:C	1	1.09
(1,618)	1:67:C:SER:C	1:68:C:LEU:N	1:68:C:LEU:CA	1:68:C:LEU:C	14	1.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	11	1.09
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	16	1.09
(1,70)	1:46:A:THR:C	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	2	1.09
(1,842)	1:54:D:ASP:C	1:55:D:VAL:N	1:55:D:VAL:CA	1:55:D:VAL:C	7	1.08
(1,829)	1:48:D:SER:N	1:48:D:SER:CA	1:48:D:SER:C	1:49:D:SER:N	9	1.08
(1,814)	1:40:D:VAL:C	1:41:D:LYS:N	1:41:D:LYS:CA	1:41:D:LYS:C	20	1.08
(1,761)	1:11:D:PHE:N	1:11:D:PHE:CA	1:11:D:PHE:C	1:12:D:GLN:N	6	1.08
(1,730)	1:126:C:LEU:C	1:127:C:ASN:N	1:127:C:ASN:CA	1:127:C:ASN:C	11	1.08
(1,620)	1:68:C:LEU:C	1:69:C:GLY:N	1:69:C:GLY:CA	1:69:C:GLY:C	6	1.08
(1,611)	1:64:C:VAL:N	1:64:C:VAL:CA	1:64:C:VAL:C	1:65:C:THR:N	9	1.08
(1,391)	1:80:B:GLN:N	1:80:B:GLN:CA	1:80:B:GLN:C	1:81:B:GLY:N	6	1.08
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	6	1.08
(1,37)	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1:29:A:PRO:N	7	1.08
(1,902)	1:84:D:PHE:C	1:85:D:SER:N	1:85:D:SER:CA	1:85:D:SER:C	7	1.07
(1,872)	1:69:D:GLY:C	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	17	1.07
(1,860)	1:63:D:THR:C	1:64:D:VAL:N	1:64:D:VAL:CA	1:64:D:VAL:C	6	1.07
(1,810)	1:38:D:PRO:C	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	11	1.07
(1,807)	1:36:D:TRP:N	1:36:D:TRP:CA	1:36:D:TRP:C	1:37:D:GLN:N	7	1.07
(1,737)	1:131:C:VAL:N	1:131:C:VAL:CA	1:131:C:VAL:C	1:132:C:ASN:N	1	1.07
(1,685)	1:101:C:TYR:N	1:101:C:TYR:CA	1:101:C:TYR:C	1:102:C:CYS:N	6	1.07
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1	1.07
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	14	1.07
(1,63)	1:43:A:ASP:N	1:43:A:ASP:CA	1:43:A:ASP:C	1:44:A:LEU:N	9	1.07
(1,34)	1:26:A:PRO:C	1:27:A:ASN:N	1:27:A:ASN:CA	1:27:A:ASN:C	9	1.07
(1,856)	1:61:D:ARG:C	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	12	1.06
(1,727)	1:125:C:GLN:N	1:125:C:GLN:CA	1:125:C:GLN:C	1:126:C:LEU:N	1	1.06
(1,369)	1:69:B:GLY:N	1:69:B:GLY:CA	1:69:B:GLY:C	1:70:B:GLU:N	14	1.06
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	2	1.06
(1,95)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:LEU:N	2	1.06
(1,980)	1:126:D:LEU:C	1:127:D:ASN:N	1:127:D:ASN:CA	1:127:D:ASN:C	14	1.05
(1,855)	1:61:D:ARG:N	1:61:D:ARG:CA	1:61:D:ARG:C	1:62:D:VAL:N	14	1.05
(1,786)	1:23:D:PHE:C	1:24:D:GLU:N	1:24:D:GLU:CA	1:24:D:GLU:C	12	1.05
(1,770)	1:15:D:ARG:C	1:16:D:ILE:N	1:16:D:ILE:CA	1:16:D:ILE:C	15	1.05
(1,595)	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1:57:C:GLU:N	8	1.05
(1,591)	1:54:C:ASP:N	1:54:C:ASP:CA	1:54:C:ASP:C	1:55:C:VAL:N	2	1.05
(1,323)	1:46:B:THR:N	1:46:B:THR:CA	1:46:B:THR:C	1:47:B:ALA:N	16	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
(1,37)	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	1:29:A:PRO:N	3	1.05
(1,985)	1:129:D:ALA:N	1:129:D:ALA:CA	1:129:D:ALA:C	1:130:D:PRO:N	9	1.04
(1,931)	1:99:D:GLY:N	1:99:D:GLY:CA	1:99:D:GLY:C	1:100:D:ALA:N	20	1.04
(1,873)	1:70:D:GLU:N	1:70:D:GLU:CA	1:70:D:GLU:C	1:71:D:GLU:N	1	1.04
(1,761)	1:11:D:PHE:N	1:11:D:PHE:CA	1:11:D:PHE:C	1:12:D:GLN:N	2	1.04
(1,682)	1:99:C:GLY:C	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	11	1.04
(1,305)	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1:37:B:GLN:N	2	1.04
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	16	1.04
(1,113)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLY:N	2	1.04
(1,112)	1:67:A:SER:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	18	1.04
(1,3)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:PHE:N	20	1.04
(1,1008)	1:141:D:LEU:C	1:142:D:GLN:N	1:142:D:GLN:CA	1:142:D:GLN:C	18	1.03
(1,762)	1:11:D:PHE:C	1:12:D:GLN:N	1:12:D:GLN:CA	1:12:D:GLN:C	13	1.03
(1,749)	1:137:C:PHE:N	1:137:C:PHE:CA	1:137:C:PHE:C	1:138:C:MET:N	3	1.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,657)	1:87:C:ALA:N	1:87:C:ALA:CA	1:87:C:ALA:C	1:88:C:GLY:N	3	1.03
(1,598)	1:57:C:GLU:C	1:58:C:VAL:N	1:58:C:VAL:CA	1:58:C:VAL:C	3	1.03
(1,512)	1:11:C:PHE:C	1:12:C:GLN:N	1:12:C:GLN:CA	1:12:C:GLN:C	10	1.03
(1,484)	1:130:B:PRO:C	1:131:B:VAL:N	1:131:B:VAL:CA	1:131:B:VAL:C	7	1.03
(1,425)	1:97:B:CYS:N	1:97:B:CYS:CA	1:97:B:CYS:C	1:98:B:LEU:N	13	1.03
(1,175)	1:99:A:GLY:N	1:99:A:GLY:CA	1:99:A:GLY:C	1:100:A:ALA:N	5	1.03
(1,164)	1:93:A:GLN:C	1:94:A:MET:N	1:94:A:MET:CA	1:94:A:MET:C	20	1.03
(1,102)	1:62:A:VAL:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	10	1.03
(1,74)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	3	1.03
(1,54)	1:38:A:PRO:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1	1.03
(1,47)	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1:35:A:ASP:N	12	1.03
(1,18)	1:17:A:TYR:C	1:18:A:THR:N	1:18:A:THR:CA	1:18:A:THR:C	3	1.03
(1,926)	1:96:D:HIS:C	1:97:D:CYS:N	1:97:D:CYS:CA	1:97:D:CYS:C	12	1.02
(1,856)	1:61:D:ARG:C	1:62:D:VAL:N	1:62:D:VAL:CA	1:62:D:VAL:C	9	1.02
(1,683)	1:100:C:ALA:N	1:100:C:ALA:CA	1:100:C:ALA:C	1:101:C:TYR:N	9	1.02
(1,594)	1:55:C:VAL:C	1:56:C:TYR:N	1:56:C:TYR:CA	1:56:C:TYR:C	1	1.02
(1,481)	1:128:B:LEU:N	1:128:B:LEU:CA	1:128:B:LEU:C	1:129:B:ALA:N	7	1.02
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	5	1.02
(1,327)	1:48:B:SER:N	1:48:B:SER:CA	1:48:B:SER:C	1:49:B:SER:N	16	1.02
(1,271)	1:17:B:TYR:N	1:17:B:TYR:CA	1:17:B:TYR:C	1:18:B:THR:N	3	1.02
(1,36)	1:27:A:ASN:C	1:28:A:ALA:N	1:28:A:ALA:CA	1:28:A:ALA:C	17	1.02
(1,886)	1:76:D:CYS:C	1:77:D:GLU:N	1:77:D:GLU:CA	1:77:D:GLU:C	17	1.01
(1,811)	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	1:40:D:VAL:N	17	1.01
(1,769)	1:15:D:ARG:N	1:15:D:ARG:CA	1:15:D:ARG:C	1:16:D:ILE:N	20	1.01
(1,658)	1:87:C:ALA:C	1:88:C:GLY:N	1:88:C:GLY:CA	1:88:C:GLY:C	4	1.01
(1,511)	1:11:C:PHE:N	1:11:C:PHE:CA	1:11:C:PHE:C	1:12:C:GLN:N	6	1.01
(1,340)	1:54:B:ASP:C	1:55:B:VAL:N	1:55:B:VAL:CA	1:55:B:VAL:C	5	1.01
(1,331)	1:50:B:GLN:N	1:50:B:GLN:CA	1:50:B:GLN:C	1:51:B:LEU:N	12	1.01
(1,268)	1:15:B:ARG:C	1:16:B:ILE:N	1:16:B:ILE:CA	1:16:B:ILE:C	11	1.01
(1,57)	1:40:A:VAL:N	1:40:A:VAL:CA	1:40:A:VAL:C	1:41:A:LYS:N	3	1.01
(1,845)	1:56:D:TYR:N	1:56:D:TYR:CA	1:56:D:TYR:C	1:57:D:GLU:N	19	1.0
(1,810)	1:38:D:PRO:C	1:39:D:GLU:N	1:39:D:GLU:CA	1:39:D:GLU:C	5	1.0
(1,642)	1:79:C:GLN:C	1:80:C:GLN:N	1:80:C:GLN:CA	1:80:C:GLN:C	2	1.0
(1,399)	1:84:B:PHE:N	1:84:B:PHE:CA	1:84:B:PHE:C	1:85:B:SER:N	16	1.0
(1,393)	1:81:B:GLY:N	1:81:B:GLY:CA	1:81:B:GLY:C	1:82:B:GLY:N	14	1.0
(1,305)	1:36:B:TRP:N	1:36:B:TRP:CA	1:36:B:TRP:C	1:37:B:GLN:N	7	1.0