



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 01:00 PM UTC

PDB ID : 2M03 / pdb_00002m03
BMRB ID : 18792
Title : Solution structure of BCL-xL determined with selective isotope labelling of I,L,V sidechains
Authors : Viacava Follis, A.; Royappa, G.; Kriwacki, R.W.
Deposited on : 2012-10-19

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 ⓘ 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 ⓘ](#)) 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

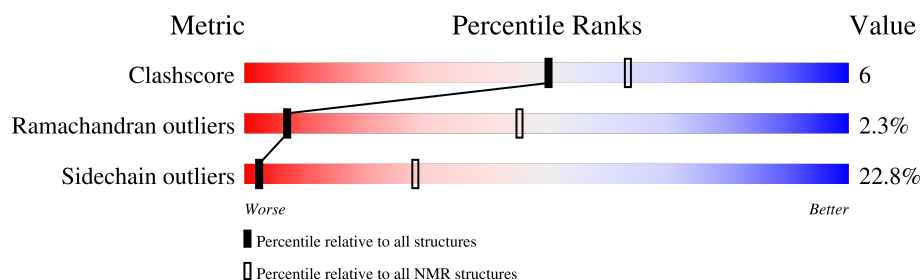
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	181	

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:26, A:47-A:78, A:83-A:159 (131)	1.35	1

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2764 atoms, of which 1338 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	177	Total	C	H	N	O	S	0
			2764	894	1338	246	280	6	

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q07817
A	2	SER	-	expression tag	UNP Q07817
A	3	MET	-	expression tag	UNP Q07817
A	4	ALA	-	expression tag	UNP Q07817
A	?	-	MET	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	TRP	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ASP	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ASN	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	THR	deletion	UNP Q07817
A	?	-	GLY	deletion	UNP Q07817
A	?	-	HIS	deletion	UNP Q07817

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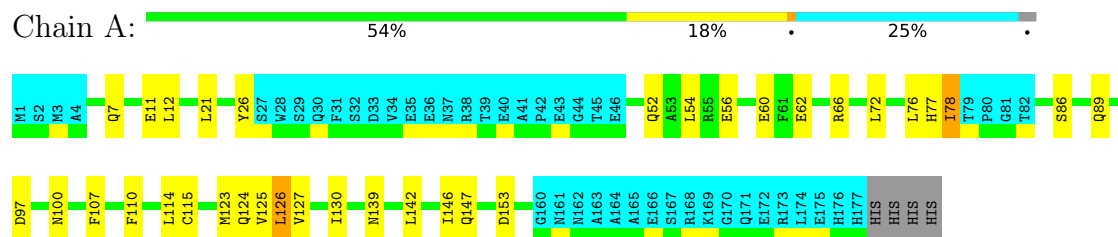
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	SER	deletion	UNP Q07817
A	?	-	LEU	deletion	UNP Q07817
A	?	-	ASP	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	?	-	ARG	deletion	UNP Q07817
A	?	-	GLU	deletion	UNP Q07817
A	?	-	VAL	deletion	UNP Q07817
A	?	-	ILE	deletion	UNP Q07817
A	?	-	PRO	deletion	UNP Q07817
A	?	-	MET	deletion	UNP Q07817
A	?	-	ALA	deletion	UNP Q07817
A	174	LEU	-	expression tag	UNP Q07817
A	175	GLU	-	expression tag	UNP Q07817
A	176	HIS	-	expression tag	UNP Q07817
A	177	HIS	-	expression tag	UNP Q07817
A	178	HIS	-	expression tag	UNP Q07817
A	179	HIS	-	expression tag	UNP Q07817
A	180	HIS	-	expression tag	UNP Q07817
A	181	HIS	-	expression tag	UNP Q07817

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: Bcl-2-like protein 1

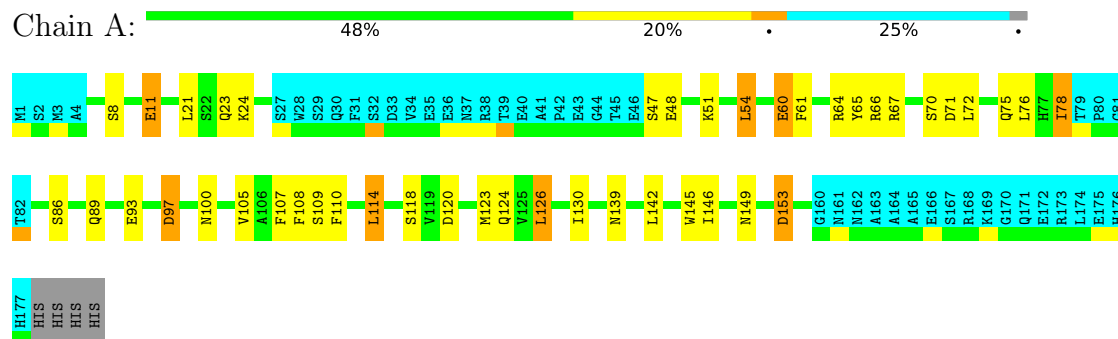


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

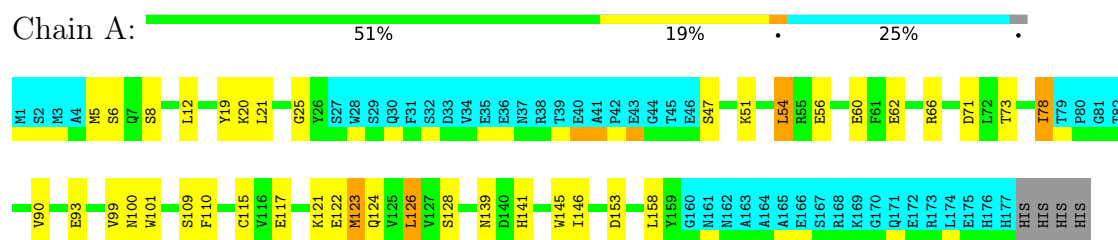
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Bcl-2-like protein 1



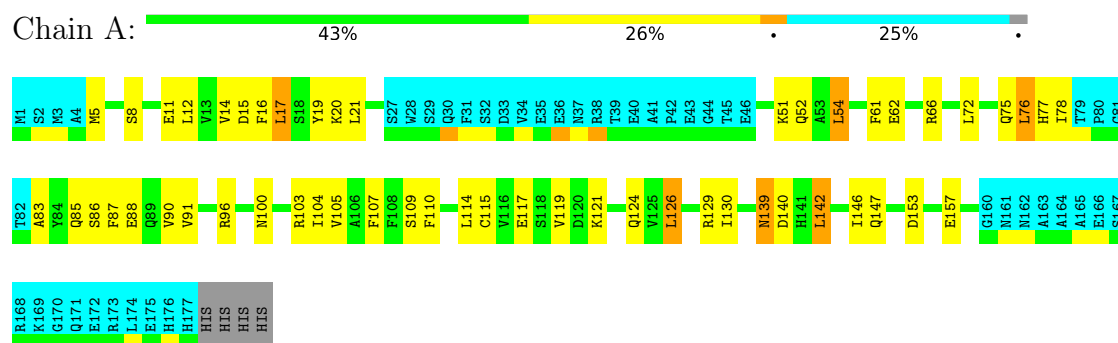
4.2.2 Score per residue for model 2

- Molecule 1: Bcl-2-like protein 1



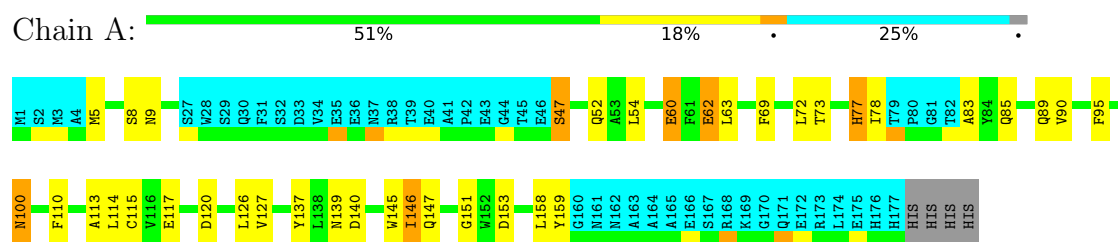
4.2.3 Score per residue for model 3

- Molecule 1: Bcl-2-like protein 1



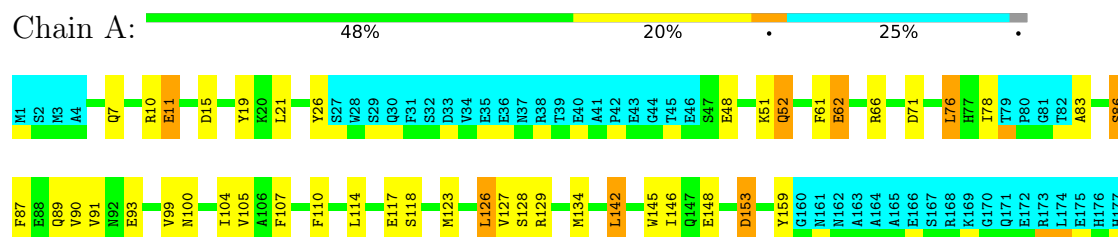
4.2.4 Score per residue for model 4

- Molecule 1: Bcl-2-like protein 1



4.2.5 Score per residue for model 5

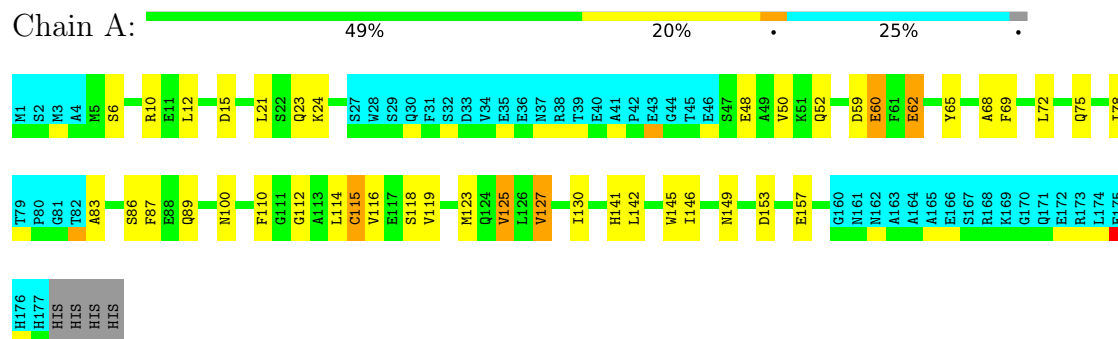
- Molecule 1: Bcl-2-like protein 1



HIS
HIS
HIS
HIS

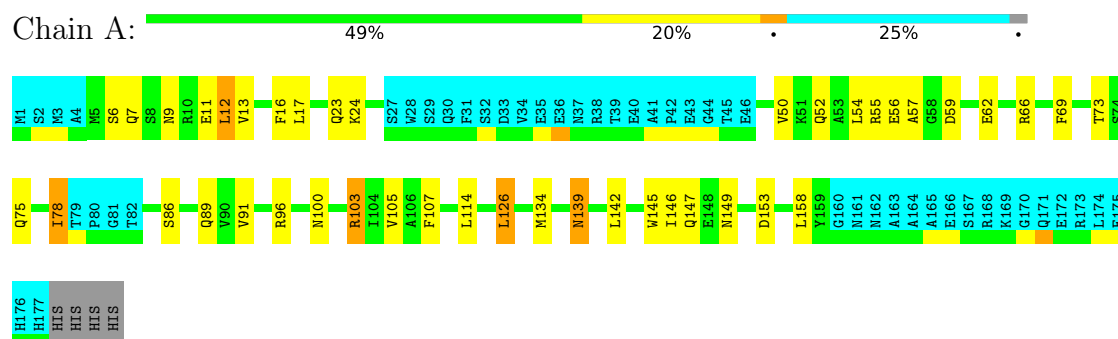
4.2.6 Score per residue for model 6

- Molecule 1: Bcl-2-like protein 1



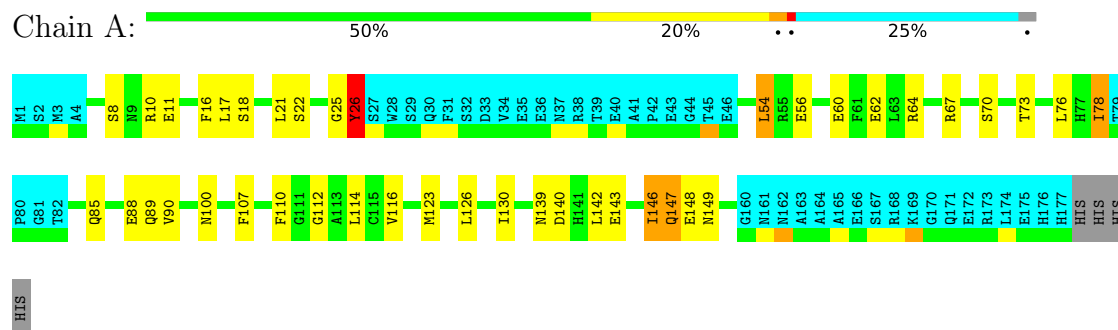
4.2.7 Score per residue for model 7

- Molecule 1: Bcl-2-like protein 1



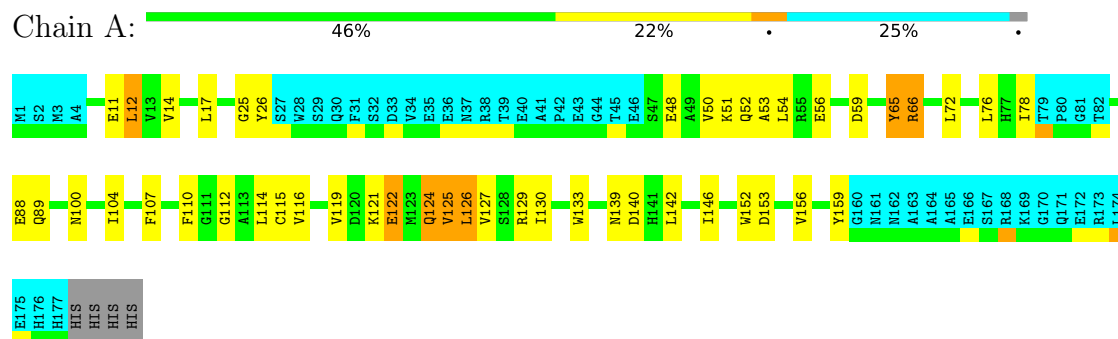
4.2.8 Score per residue for model 8

- Molecule 1: Bcl-2-like protein 1



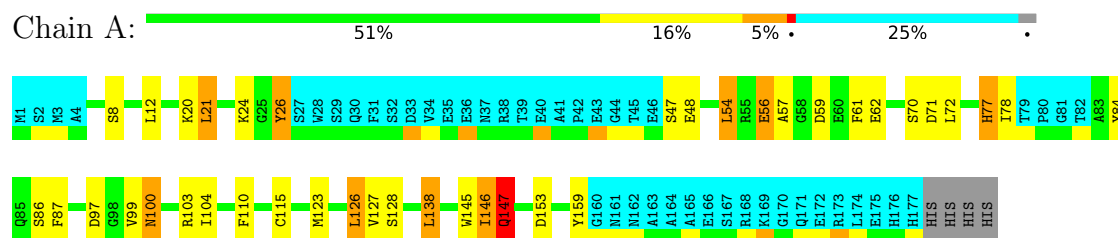
4.2.9 Score per residue for model 9

- Molecule 1: Bcl-2-like protein 1



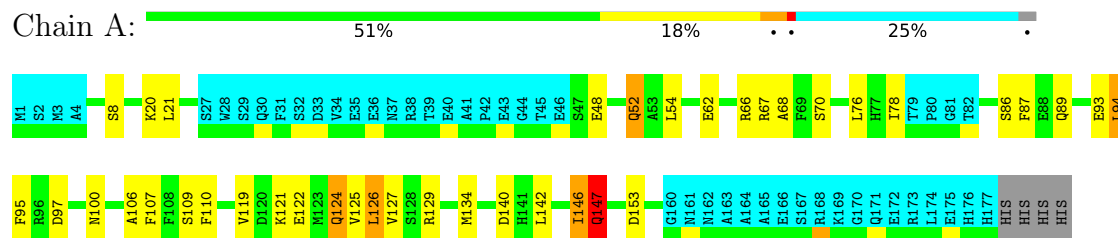
4.2.10 Score per residue for model 10

- Molecule 1: Bcl-2-like protein 1



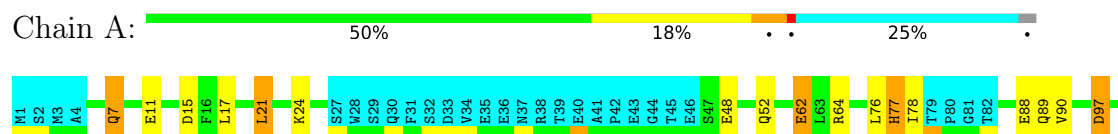
4.2.11 Score per residue for model 11

- Molecule 1: Bcl-2-like protein 1



4.2.12 Score per residue for model 12

- Molecule 1: Bcl-2-like protein 1

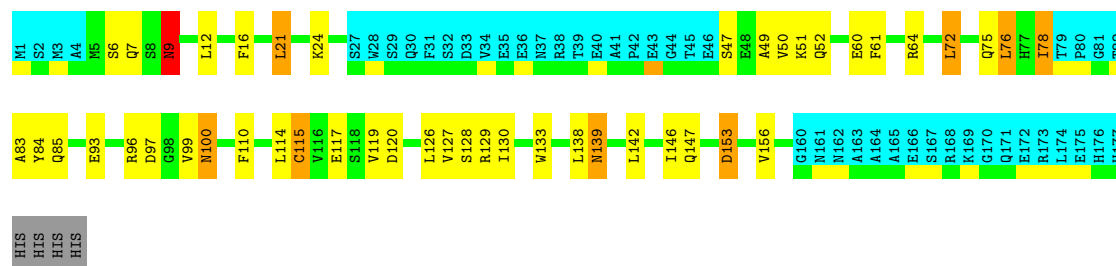




4.2.13 Score per residue for model 13

- Molecule 1: Bcl-2-like protein 1

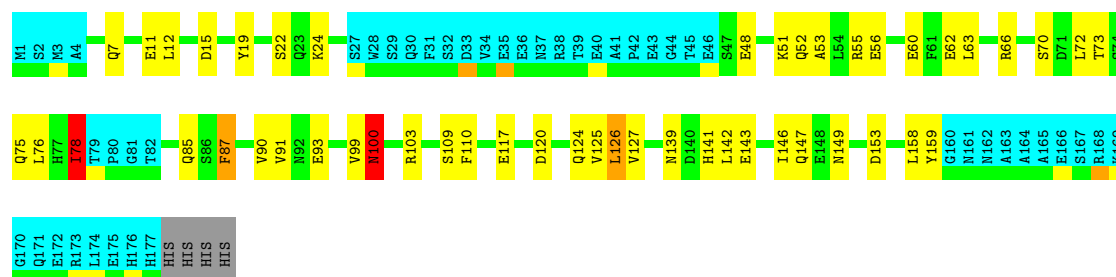
Chain A: 47% 20% 25%



4.2.14 Score per residue for model 14

- Molecule 1: Bcl-2-like protein 1

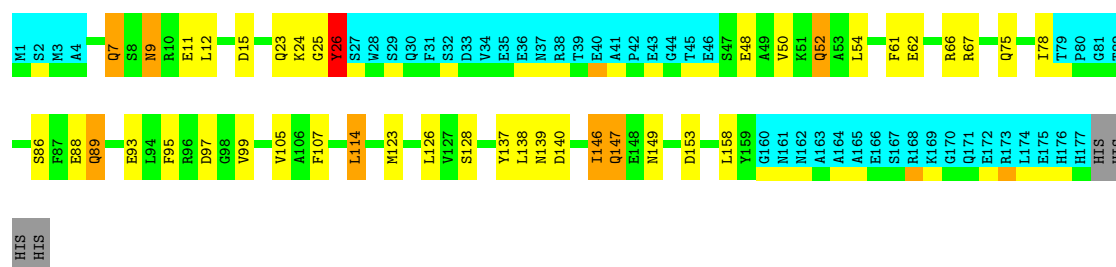
Chain A: 45% 25% 25%



4.2.15 Score per residue for model 15

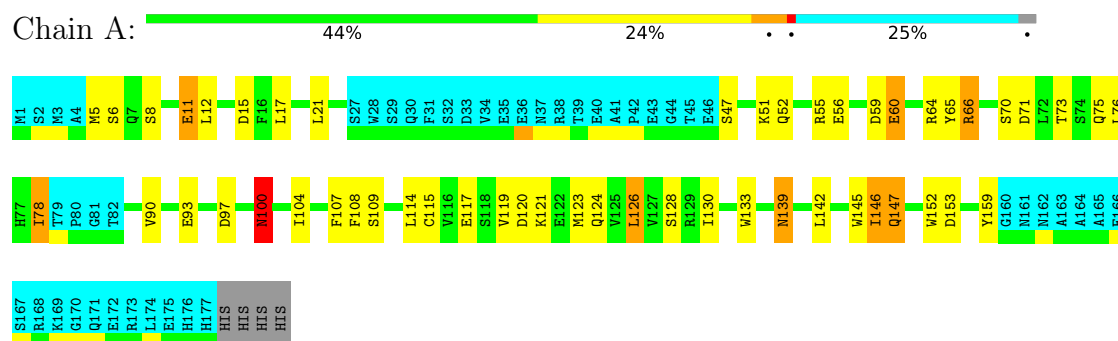
- Molecule 1: Bcl-2-like protein 1

Chain A: 50% 18% 25%



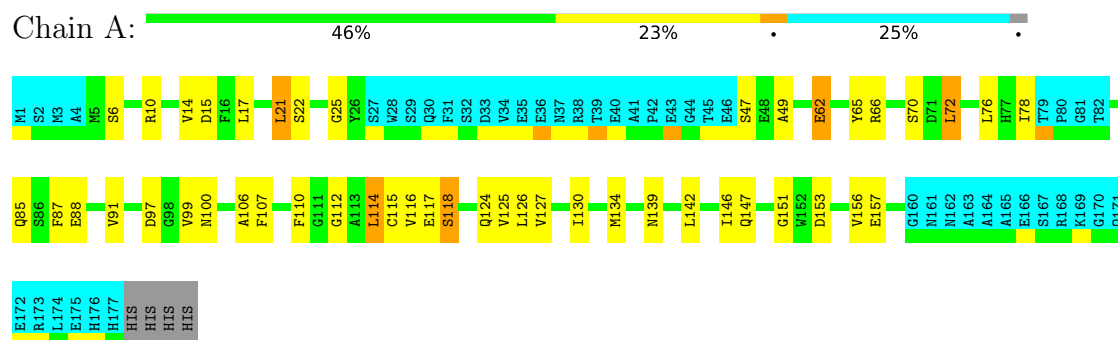
4.2.16 Score per residue for model 16

- Molecule 1: Bcl-2-like protein 1



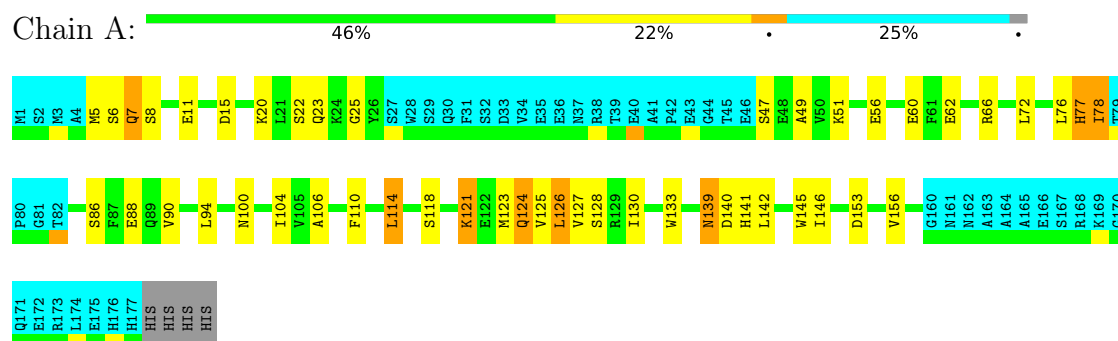
4.2.17 Score per residue for model 17

- Molecule 1: Bcl-2-like protein 1



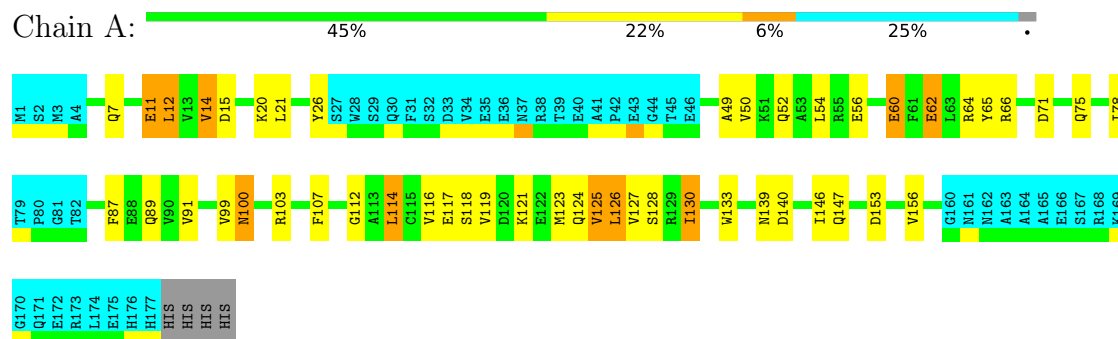
4.2.18 Score per residue for model 18

- Molecule 1: Bcl-2-like protein 1



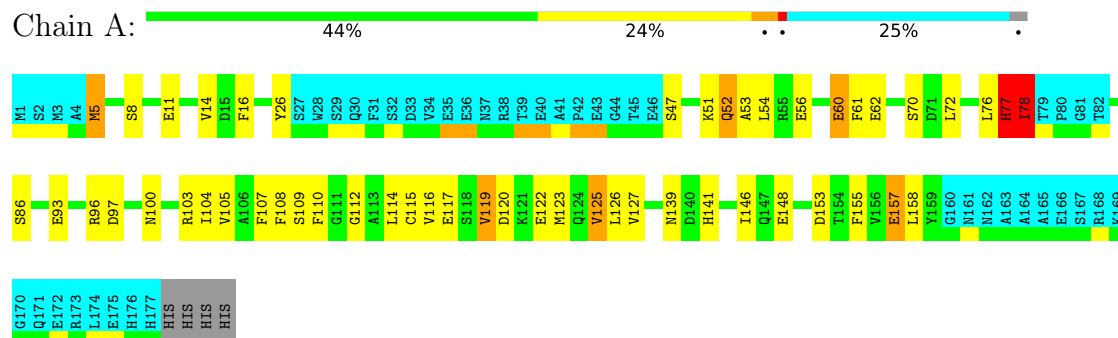
4.2.19 Score per residue for model 19

- Molecule 1: Bcl-2-like protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Bcl-2-like protein 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle simulated annealing, molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1050
Number of shifts mapped to atoms	1050
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

6 Model quality i

6.1 Standard geometry i

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	0.71±0.02	0±0/1099 (0.0± 0.0%)	1.22±0.02	2±1/1487 (0.2± 0.1%)
All	All	0.71	0/21980 (0.0%)	1.22	48/29740 (0.2%)

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	A	0.0±0.0	6.0±1.9
All	All	0	120

There are no bond-length outliers.

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	GLN	OE1-CD-NE2	-7.62	114.98	122.60	5	9
1	A	139	ASN	OD1-CG-ND2	-7.38	115.22	122.60	3	11
1	A	124	GLN	OE1-CD-NE2	-6.73	115.87	122.60	16	3
1	A	147	GLN	OE1-CD-NE2	-6.53	116.07	122.60	11	5
1	A	23	GLN	OE1-CD-NE2	-6.25	116.35	122.60	18	4
1	A	89	GLN	OE1-CD-NE2	-6.24	116.36	122.60	15	3
1	A	9	ASN	OD1-CG-ND2	-6.23	116.37	122.60	13	3
1	A	7	GLN	OE1-CD-NE2	-5.96	116.64	122.60	15	3
1	A	78	ILE	O-C-N	5.77	126.42	121.98	2	1
1	A	77	HIS	CB-CG-CD2	-5.23	124.40	131.20	12	1
1	A	75	GLN	OE1-CD-NE2	-5.13	117.47	122.60	3	4
1	A	100	ASN	OD1-CG-ND2	-5.01	117.58	122.60	8	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	11	GLU	Mainchain,Sidechain	13
1	A	100	ASN	Mainchain	13
1	A	62	GLU	Sidechain	11
1	A	60	GLU	Sidechain	10
1	A	15	ASP	Sidechain,Mainchain	10
1	A	56	GLU	Sidechain,Mainchain	5
1	A	59	ASP	Mainchain,Sidechain	5
1	A	65	TYR	Mainchain,Sidechain	4
1	A	153	ASP	Mainchain,Sidechain	4
1	A	26	TYR	Sidechain,Mainchain	4
1	A	120	ASP	Sidechain	3
1	A	66	ARG	Mainchain	3
1	A	48	GLU	Sidechain	3
1	A	97	ASP	Sidechain	3
1	A	7	GLN	Mainchain	2
1	A	157	GLU	Sidechain	2
1	A	121	LYS	Mainchain	2
1	A	64	ARG	Mainchain	1
1	A	124	GLN	Mainchain	1
1	A	25	GLY	Mainchain	1
1	A	140	ASP	Sidechain	1
1	A	71	ASP	Sidechain	1
1	A	159	TYR	Sidechain	1
1	A	52	GLN	Mainchain	1
1	A	18	SER	Mainchain	1
1	A	21	LEU	Mainchain	1
1	A	84	TYR	Mainchain	1
1	A	122	GLU	Sidechain	1
1	A	147	GLN	Sidechain	1
1	A	67	ARG	Mainchain	1
1	A	93	GLU	Sidechain	1
1	A	5	MET	Mainchain	1
1	A	117	GLU	Sidechain	1
1	A	119	VAL	Mainchain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1073	1023	1023	12±3
All	All	21460	20460	20460	236

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD21	1:A:130:ILE:HD12	0.86	1.45	18	1
1:A:76:LEU:HD21	1:A:114:LEU:HD23	0.83	1.48	3	1
1:A:114:LEU:HD21	1:A:130:ILE:HD13	0.81	1.50	17	2
1:A:78:ILE:HD11	1:A:126:LEU:HD11	0.80	1.52	5	5
1:A:107:PHE:CE2	1:A:138:LEU:HD13	0.71	2.20	15	1
1:A:78:ILE:HD11	1:A:126:LEU:HD12	0.69	1.64	20	1
1:A:78:ILE:HD11	1:A:126:LEU:HD21	0.68	1.64	19	6
1:A:114:LEU:HD23	1:A:130:ILE:HD13	0.68	1.65	1	1
1:A:114:LEU:HD12	1:A:130:ILE:CD1	0.67	2.19	3	1
1:A:49:ALA:HB1	1:A:156:VAL:HG22	0.67	1.66	18	1
1:A:124:GLN:HB3	1:A:126:LEU:HD22	0.65	1.66	11	2
1:A:106:ALA:HB1	1:A:110:PHE:CE2	0.64	2.28	11	1
1:A:16:PHE:CE2	1:A:54:LEU:HD22	0.63	2.28	3	2
1:A:126:LEU:HD13	1:A:127:VAL:N	0.63	2.09	10	1
1:A:53:ALA:HB1	1:A:155:PHE:CD1	0.63	2.29	20	1
1:A:100:ASN:HA	1:A:104:ILE:HD12	0.62	1.70	20	4
1:A:76:LEU:HD22	1:A:110:PHE:CE1	0.62	2.29	3	1
1:A:78:ILE:HD11	1:A:126:LEU:HD13	0.61	1.71	15	1
1:A:90:VAL:HG21	1:A:110:PHE:CD2	0.60	2.31	2	3
1:A:90:VAL:HG21	1:A:110:PHE:CE2	0.59	2.32	8	1
1:A:119:VAL:HG13	1:A:127:VAL:HG21	0.59	1.75	13	1
1:A:126:LEU:HD22	1:A:126:LEU:C	0.59	2.21	10	1
1:A:21:LEU:HD12	1:A:115:CYS:HB3	0.59	1.74	17	1
1:A:78:ILE:CD1	1:A:114:LEU:HD11	0.59	2.28	3	2
1:A:12:LEU:HD21	1:A:50:VAL:HG11	0.59	1.74	7	1
1:A:114:LEU:HD12	1:A:130:ILE:HD13	0.57	1.74	3	1
1:A:78:ILE:HB	1:A:114:LEU:HD11	0.57	1.76	8	2
1:A:114:LEU:CD1	1:A:130:ILE:HD12	0.57	2.29	13	1
1:A:26:TYR:CE1	1:A:119:VAL:HG11	0.57	2.35	9	2
1:A:78:ILE:HD11	1:A:126:LEU:HD22	0.57	1.76	17	2
1:A:68:ALA:HB3	1:A:110:PHE:CZ	0.57	2.35	11	1
1:A:104:ILE:HD11	1:A:142:LEU:CD1	0.56	2.31	5	2
1:A:90:VAL:HG11	1:A:110:PHE:CD2	0.56	2.35	18	1
1:A:123:MET:HB3	1:A:126:LEU:HD23	0.56	1.77	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD21	1:A:50:VAL:HG12	0.56	1.77	6	1
1:A:95:PHE:CE1	1:A:99:VAL:HG23	0.56	2.36	15	1
1:A:107:PHE:CZ	1:A:134:MET:HE3	0.55	2.36	11	1
1:A:94:LEU:HD22	1:A:106:ALA:CB	0.55	2.32	18	1
1:A:12:LEU:HD13	1:A:50:VAL:HG12	0.55	1.77	15	1
1:A:78:ILE:HG22	1:A:114:LEU:HD11	0.54	1.79	5	1
1:A:146:ILE:HD12	1:A:147:GLN:N	0.54	2.17	12	1
1:A:114:LEU:CD2	1:A:130:ILE:HD13	0.54	2.33	19	3
1:A:110:PHE:CZ	1:A:114:LEU:HD11	0.54	2.38	12	2
1:A:114:LEU:HD23	1:A:115:CYS:N	0.54	2.18	17	1
1:A:53:ALA:HB2	1:A:159:TYR:HB2	0.54	1.80	14	2
1:A:78:ILE:HD11	1:A:126:LEU:CD1	0.54	2.33	15	5
1:A:126:LEU:HD22	1:A:126:LEU:O	0.53	2.04	10	1
1:A:104:ILE:HD11	1:A:142:LEU:HD12	0.53	1.81	5	1
1:A:78:ILE:CD1	1:A:126:LEU:HD21	0.53	2.34	14	2
1:A:77:HIS:O	1:A:114:LEU:HD23	0.53	2.03	20	1
1:A:61:PHE:CG	1:A:105:VAL:HG11	0.53	2.39	5	3
1:A:114:LEU:CD2	1:A:130:ILE:HD12	0.53	2.29	18	1
1:A:76:LEU:HD21	1:A:114:LEU:CD2	0.53	2.29	3	1
1:A:72:LEU:HD13	1:A:110:PHE:HB2	0.53	1.80	6	1
1:A:78:ILE:HD13	1:A:114:LEU:HD11	0.52	1.80	3	2
1:A:76:LEU:HD13	1:A:110:PHE:CE1	0.52	2.39	20	2
1:A:72:LEU:HD22	1:A:110:PHE:CD1	0.52	2.39	17	1
1:A:115:CYS:SG	1:A:127:VAL:HG13	0.52	2.44	9	1
1:A:78:ILE:CG2	1:A:114:LEU:HD11	0.52	2.34	5	1
1:A:61:PHE:CD2	1:A:105:VAL:HG11	0.52	2.40	3	1
1:A:124:GLN:HB2	1:A:126:LEU:HD22	0.52	1.81	18	1
1:A:49:ALA:HB3	1:A:156:VAL:HG22	0.52	1.80	13	1
1:A:12:LEU:HD11	1:A:54:LEU:HD22	0.51	1.81	15	1
1:A:54:LEU:HD21	1:A:108:PHE:CE2	0.51	2.41	1	1
1:A:12:LEU:HD21	1:A:50:VAL:CG1	0.51	2.36	6	3
1:A:78:ILE:HD13	1:A:126:LEU:HD21	0.51	1.82	10	1
1:A:90:VAL:HG21	1:A:110:PHE:CE1	0.50	2.40	3	1
1:A:87:PHE:O	1:A:91:VAL:HG23	0.50	2.06	14	4
1:A:21:LEU:HD11	1:A:119:VAL:HG21	0.50	1.84	19	1
1:A:126:LEU:HD12	1:A:127:VAL:N	0.50	2.22	4	1
1:A:110:PHE:CE1	1:A:114:LEU:HD11	0.50	2.42	9	1
1:A:112:GLY:O	1:A:116:VAL:HG23	0.49	2.07	12	7
1:A:16:PHE:CD2	1:A:54:LEU:HD13	0.49	2.42	3	1
1:A:72:LEU:HD22	1:A:110:PHE:CG	0.49	2.42	13	2
1:A:78:ILE:HD13	1:A:118:SER:HB3	0.49	1.83	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:LEU:HD23	1:A:127:VAL:N	0.49	2.23	18	4
1:A:118:SER:CB	1:A:127:VAL:HG13	0.49	2.38	17	1
1:A:126:LEU:C	1:A:130:ILE:HD12	0.49	2.33	9	1
1:A:21:LEU:HD11	1:A:127:VAL:HG11	0.48	1.83	13	1
1:A:76:LEU:HD11	1:A:90:VAL:HG21	0.48	1.85	16	1
1:A:65:TYR:CE1	1:A:68:ALA:HB2	0.48	2.44	6	1
1:A:78:ILE:HD11	1:A:130:ILE:HD13	0.48	1.85	6	1
1:A:49:ALA:CB	1:A:156:VAL:HG22	0.48	2.38	13	3
1:A:78:ILE:HD11	1:A:126:LEU:CD2	0.48	2.38	17	1
1:A:17:LEU:HD22	1:A:107:PHE:CZ	0.48	2.43	16	1
1:A:49:ALA:HB1	1:A:156:VAL:HA	0.47	1.86	17	1
1:A:78:ILE:CG1	1:A:126:LEU:HD11	0.47	2.39	18	2
1:A:119:VAL:HG23	1:A:127:VAL:HG21	0.47	1.87	6	1
1:A:12:LEU:HD13	1:A:152:TRP:CZ3	0.47	2.44	9	1
1:A:115:CYS:HB2	1:A:127:VAL:HG13	0.47	1.86	13	1
1:A:126:LEU:O	1:A:130:ILE:HD12	0.47	2.09	9	1
1:A:115:CYS:O	1:A:119:VAL:HG23	0.47	2.09	3	3
1:A:78:ILE:HD11	1:A:130:ILE:HD11	0.47	1.87	8	1
1:A:16:PHE:CD1	1:A:54:LEU:HD23	0.47	2.44	20	1
1:A:78:ILE:HG13	1:A:114:LEU:HD22	0.47	1.87	12	1
1:A:126:LEU:HD13	1:A:126:LEU:C	0.47	2.35	20	1
1:A:72:LEU:HD13	1:A:110:PHE:CE2	0.46	2.45	13	1
1:A:16:PHE:CD2	1:A:54:LEU:HD23	0.46	2.45	7	1
1:A:12:LEU:HD11	1:A:50:VAL:CG1	0.46	2.40	19	2
1:A:94:LEU:HD11	1:A:95:PHE:CZ	0.46	2.46	11	1
1:A:72:LEU:HD11	1:A:90:VAL:HG13	0.46	1.86	18	1
1:A:78:ILE:CD1	1:A:114:LEU:HD22	0.46	2.40	12	1
1:A:12:LEU:C	1:A:12:LEU:HD23	0.46	2.36	16	1
1:A:78:ILE:CD1	1:A:126:LEU:HD11	0.46	2.41	11	4
1:A:75:GLN:C	1:A:76:LEU:HD22	0.46	2.36	14	1
1:A:124:GLN:HG3	1:A:127:VAL:HG23	0.46	1.86	18	1
1:A:12:LEU:HD22	1:A:152:TRP:CH2	0.45	2.46	16	1
1:A:83:ALA:HB1	1:A:87:PHE:CE2	0.45	2.46	6	1
1:A:61:PHE:CB	1:A:105:VAL:HG11	0.45	2.41	20	1
1:A:146:ILE:HD12	1:A:147:GLN:H	0.45	1.72	8	6
1:A:21:LEU:HD12	1:A:115:CYS:SG	0.45	2.52	12	1
1:A:17:LEU:HD22	1:A:134:MET:HE1	0.45	1.89	17	1
1:A:114:LEU:HD23	1:A:130:ILE:HD12	0.45	1.87	16	1
1:A:124:GLN:NE2	1:A:124:GLN:H	0.45	2.10	18	1
1:A:69:PHE:HA	1:A:72:LEU:HD12	0.45	1.88	6	1
1:A:118:SER:HB2	1:A:127:VAL:HG13	0.45	1.89	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD13	1:A:115:CYS:SG	0.44	2.52	10	3
1:A:21:LEU:HD23	1:A:22:SER:N	0.44	2.27	17	1
1:A:86:SER:O	1:A:90:VAL:HG23	0.44	2.12	3	3
1:A:115:CYS:SG	1:A:127:VAL:HG22	0.44	2.53	6	1
1:A:107:PHE:CE2	1:A:134:MET:HE3	0.44	2.47	11	1
1:A:118:SER:OG	1:A:127:VAL:HG22	0.44	2.13	19	1
1:A:78:ILE:HB	1:A:114:LEU:HD21	0.44	1.90	15	2
1:A:114:LEU:HD12	1:A:115:CYS:N	0.44	2.28	13	1
1:A:16:PHE:CD2	1:A:54:LEU:HD22	0.43	2.48	8	1
1:A:100:ASN:CA	1:A:104:ILE:HD12	0.43	2.43	9	1
1:A:110:PHE:CE1	1:A:114:LEU:HD13	0.43	2.48	1	1
1:A:50:VAL:HG22	1:A:156:VAL:CG2	0.43	2.43	9	1
1:A:57:ALA:HB1	1:A:105:VAL:HG13	0.43	1.90	7	1
1:A:17:LEU:HD11	1:A:107:PHE:CZ	0.43	2.48	9	1
1:A:100:ASN:HB2	1:A:146:ILE:HD13	0.43	1.90	12	1
1:A:95:PHE:CE1	1:A:106:ALA:HB3	0.43	2.48	11	1
1:A:115:CYS:HA	1:A:127:VAL:HG22	0.43	1.88	20	1
1:A:118:SER:OG	1:A:127:VAL:HG23	0.43	2.14	6	1
1:A:78:ILE:HD12	1:A:126:LEU:HD11	0.43	1.90	16	1
1:A:118:SER:CB	1:A:127:VAL:HG23	0.43	2.44	6	1
1:A:119:VAL:HB	1:A:127:VAL:HG21	0.43	1.91	11	1
1:A:100:ASN:CG	1:A:146:ILE:HD13	0.42	2.39	12	1
1:A:11:GLU:HA	1:A:14:VAL:HG12	0.42	1.91	19	1
1:A:106:ALA:HB1	1:A:110:PHE:CZ	0.42	2.49	17	1
1:A:100:ASN:CB	1:A:146:ILE:HD13	0.42	2.44	12	1
1:A:123:MET:O	1:A:126:LEU:HD12	0.42	2.15	10	1
1:A:72:LEU:HD12	1:A:110:PHE:CG	0.41	2.50	18	1
1:A:78:ILE:CG1	1:A:126:LEU:HD21	0.41	2.44	1	1
1:A:12:LEU:HD11	1:A:54:LEU:HD12	0.41	1.91	2	1
1:A:100:ASN:HA	1:A:104:ILE:HD13	0.41	1.91	16	1
1:A:126:LEU:HD12	1:A:126:LEU:C	0.41	2.40	4	1
1:A:87:PHE:CZ	1:A:130:ILE:HG23	0.41	2.49	17	1
1:A:123:MET:CB	1:A:126:LEU:HD23	0.41	2.46	15	1
1:A:87:PHE:O	1:A:91:VAL:HG13	0.41	2.15	19	1
1:A:69:PHE:CE1	1:A:113:ALA:HB2	0.41	2.51	4	1
1:A:138:LEU:HD23	1:A:139:ASN:N	0.41	2.31	13	1
1:A:115:CYS:HB3	1:A:127:VAL:HG13	0.41	1.93	4	1
1:A:91:VAL:HG13	1:A:103:ARG:HH11	0.41	1.75	7	1
1:A:90:VAL:HG11	1:A:110:PHE:CE2	0.41	2.51	14	1
1:A:104:ILE:HG22	1:A:108:PHE:CE2	0.41	2.51	20	1
1:A:126:LEU:HD23	1:A:126:LEU:C	0.40	2.41	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ASN:ND2	1:A:138:LEU:HD21	0.40	2.31	13	1
1:A:12:LEU:CD1	1:A:54:LEU:HD22	0.40	2.46	10	1
1:A:126:LEU:HD12	1:A:130:ILE:HG12	0.40	1.93	1	1
1:A:69:PHE:O	1:A:73:THR:HG22	0.40	2.16	7	1
1:A:13:VAL:HG12	1:A:17:LEU:HD12	0.40	1.93	7	1
1:A:72:LEU:HD22	1:A:110:PHE:CD2	0.40	2.52	10	1
1:A:94:LEU:HD11	1:A:95:PHE:CE1	0.40	2.52	11	1
1:A:104:ILE:HD12	1:A:104:ILE:N	0.40	2.32	16	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/181 (72%)	114±2 (87±2%)	14±2 (10±2%)	3±1 (2±1%)	7	45
All	All	2620/3620 (72%)	2287 (87%)	273 (10%)	60 (2%)	7	45

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	125	VAL	9
1	A	78	ILE	6
1	A	99	VAL	6
1	A	77	HIS	6
1	A	100	ASN	6
1	A	25	GLY	5
1	A	83	ALA	4
1	A	97	ASP	3
1	A	47	SER	3
1	A	122	GLU	3
1	A	151	GLY	2
1	A	148	GLU	2
1	A	26	TYR	2
1	A	138	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	159	TYR	1
1	A	66	ARG	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/154 (73%)	87±4 (77±3%)	26±4 (23±3%)	2	28
All	All	2260/3080 (73%)	1744 (77%)	516 (23%)	2	28

All 92 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	146	ILE	19
1	A	153	ASP	18
1	A	126	LEU	14
1	A	142	LEU	14
1	A	66	ARG	11
1	A	62	GLU	11
1	A	8	SER	10
1	A	51	LYS	10
1	A	76	LEU	10
1	A	147	GLN	10
1	A	21	LEU	9
1	A	54	LEU	9
1	A	89	GLN	9
1	A	145	TRP	9
1	A	117	GLU	9
1	A	24	LYS	8
1	A	70	SER	8
1	A	72	LEU	8
1	A	86	SER	8
1	A	93	GLU	8
1	A	107	PHE	8
1	A	109	SER	8
1	A	123	MET	8

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Mol	Chain	Res	Type	Models (Total)
1	A	128	SER	8
1	A	139	ASN	8
1	A	140	ASP	8
1	A	52	GLN	8
1	A	47	SER	7
1	A	60	GLU	7
1	A	114	LEU	7
1	A	6	SER	7
1	A	121	LYS	7
1	A	124	GLN	7
1	A	88	GLU	7
1	A	48	GLU	6
1	A	149	ASN	6
1	A	5	MET	6
1	A	20	LYS	6
1	A	85	GLN	6
1	A	103	ARG	6
1	A	7	GLN	6
1	A	56	GLU	6
1	A	71	ASP	5
1	A	97	ASP	5
1	A	73	THR	5
1	A	141	HIS	5
1	A	12	LEU	5
1	A	14	VAL	5
1	A	129	ARG	5
1	A	158	LEU	5
1	A	64	ARG	5
1	A	133	TRP	5
1	A	118	SER	4
1	A	19	TYR	4
1	A	96	ARG	4
1	A	77	HIS	4
1	A	159	TYR	4
1	A	10	ARG	4
1	A	26	TYR	4
1	A	75	GLN	4
1	A	125	VAL	4
1	A	78	ILE	4
1	A	11	GLU	3
1	A	67	ARG	3
1	A	120	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	17	LEU	3
1	A	157	GLU	3
1	A	134	MET	3
1	A	9	ASN	3
1	A	55	ARG	3
1	A	22	SER	3
1	A	143	GLU	3
1	A	87	PHE	3
1	A	100	ASN	3
1	A	122	GLU	2
1	A	63	LEU	2
1	A	137	TYR	2
1	A	115	CYS	2
1	A	65	TYR	2
1	A	61	PHE	2
1	A	130	ILE	2
1	A	23	GLN	1
1	A	95	PHE	1
1	A	127	VAL	1
1	A	148	GLU	1
1	A	104	ILE	1
1	A	138	LEU	1
1	A	94	LEU	1
1	A	16	PHE	1
1	A	84	TYR	1
1	A	108	PHE	1
1	A	99	VAL	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

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1050
Number of shifts mapped to atoms	1050
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	164	-0.14 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	151	1.36 ± 0.06	Should be checked
$^{13}\text{C}'$	164	-0.49 ± 0.06	None needed (< 0.5 ppm)
^{15}N	166	0.62 ± 0.15	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 46%, i.e. 849 atoms were assigned a chemical shift out of a possible 1829. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	508/661 (77%)	127/269 (47%)	254/262 (97%)	127/130 (98%)
Sidechain	333/960 (35%)	162/622 (26%)	171/297 (58%)	0/41 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	8/208 (4%)	4/101 (4%)	0/99 (0%)	4/8 (50%)
Overall	849/1829 (46%)	293/992 (30%)	425/658 (65%)	131/179 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 1048 atoms were assigned a chemical shift out of a possible 2396. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	656/891 (74%)	164/363 (45%)	328/354 (93%)	164/174 (94%)
Sidechain	382/1260 (30%)	174/812 (21%)	208/392 (53%)	0/56 (0%)
Aromatic	10/245 (4%)	5/120 (4%)	0/113 (0%)	5/12 (42%)
Overall	1048/2396 (44%)	343/1295 (26%)	536/859 (62%)	169/242 (70%)

7.1.4 Statistically unusual chemical shifts [i](#)

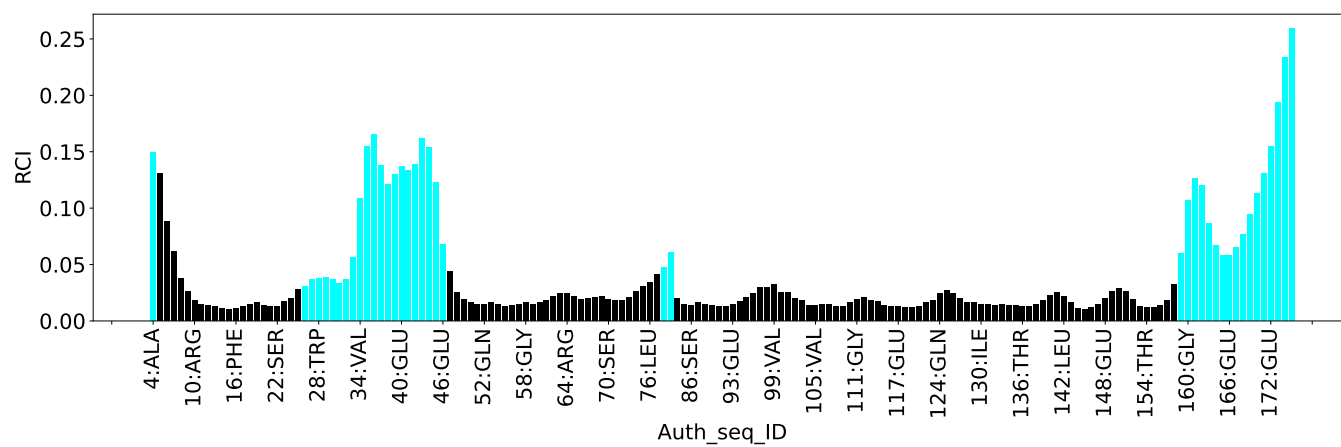
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	99	VAL	HG21	-0.82	-0.58 – 2.19	-5.9
1	A	99	VAL	HG22	-0.82	-0.58 – 2.19	-5.9
1	A	99	VAL	HG23	-0.82	-0.58 – 2.19	-5.9

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	521
Intra-residue ($ i-j =0$)	40
Sequential ($ i-j =1$)	188
Medium range ($ i-j >1$ and $ i-j <5$)	184
Long range ($ i-j \geq 5$)	109
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	247
Number of unmapped restraints	0
Number of restraints per residue	4.2
Number of long range restraints per residue ¹	0.6

¹Long 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)	38.5	0.2
0.2-0.5 (Medium)	58.4	0.5
>0.5 (Large)	31.1	4.81

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)	15.8	9.99
10.0-20.0 (Medium)	3.4	19.83
>20.0 (Large)	8.6	155.42

9 Distance violation analysis ⓘ

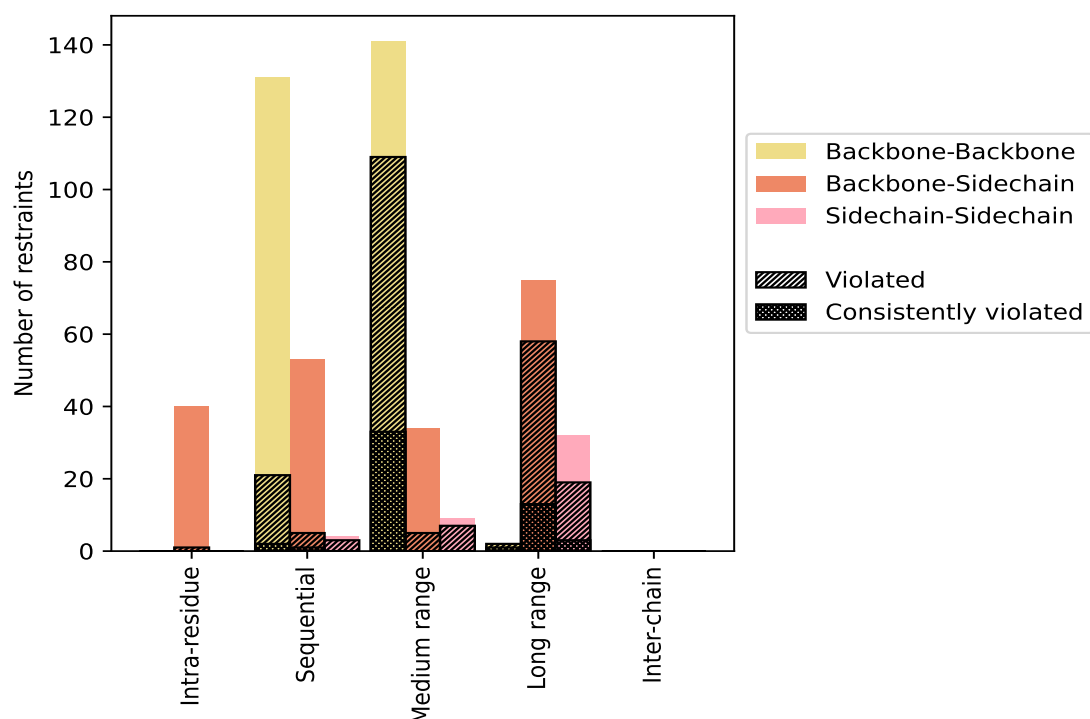
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	40	7.7	1	2.5	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	40	7.7	1	2.5	0.2	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	188	36.1	29	15.4	5.6	3	1.6	0.6
Backbone-Backbone	131	25.1	21	16.0	4.0	2	1.5	0.4
Backbone-Sidechain	53	10.2	5	9.4	1.0	1	1.9	0.2
Sidechain-Sidechain	4	0.8	3	75.0	0.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	184	35.3	121	65.8	23.2	33	17.9	6.3
Backbone-Backbone	141	27.1	109	77.3	20.9	33	23.4	6.3
Backbone-Sidechain	34	6.5	5	14.7	1.0	0	0.0	0.0
Sidechain-Sidechain	9	1.7	7	77.8	1.3	0	0.0	0.0
Long range ($i-j \geq 5$)	109	20.9	79	72.5	15.2	17	15.6	3.3
Backbone-Backbone	2	0.4	2	100.0	0.4	1	50.0	0.2
Backbone-Sidechain	75	14.4	58	77.3	11.1	13	17.3	2.5
Sidechain-Sidechain	32	6.1	19	59.4	3.6	3	9.4	0.6
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	521	100.0	230	44.1	44.1	53	10.2	10.2
Backbone-Backbone	274	52.6	132	48.2	25.3	36	13.1	6.9
Backbone-Sidechain	202	38.8	69	34.2	13.2	14	6.9	2.7
Sidechain-Sidechain	45	8.6	29	64.4	5.6	3	6.7	0.6

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 [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	9	80	36	0	126	0.44	4.81	0.58	0.28
2	1	8	77	45	0	131	0.46	3.55	0.51	0.3
3	1	9	76	42	0	128	0.46	3.25	0.51	0.3
4	1	6	79	38	0	124	0.46	4.04	0.51	0.29
5	1	8	79	39	0	127	0.44	3.24	0.47	0.29
6	1	9	75	42	0	127	0.43	3.19	0.47	0.29
7	1	8	78	46	0	133	0.46	4.39	0.52	0.3
8	1	10	85	48	0	144	0.42	4.26	0.49	0.28
9	0	10	77	46	0	133	0.45	4.6	0.5	0.29
10	0	7	76	40	0	123	0.42	3.32	0.47	0.25

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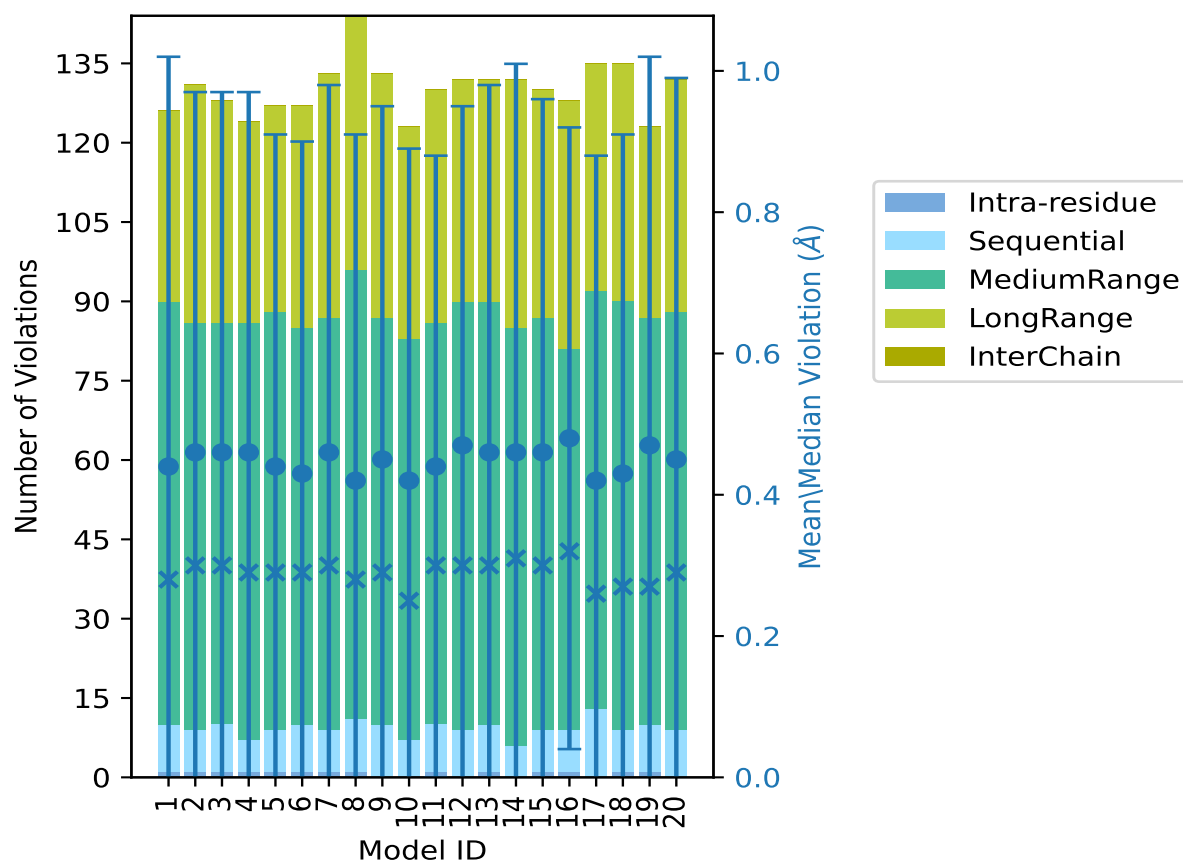
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	9	76	44	0	130	0.44	2.82	0.44	0.3
12	0	9	81	42	0	132	0.47	3.55	0.48	0.3
13	1	9	80	42	0	132	0.46	4.03	0.52	0.3
14	0	6	79	47	0	132	0.46	4.49	0.55	0.31
15	1	8	78	43	0	130	0.46	3.76	0.5	0.3
16	1	8	72	47	0	128	0.48	2.9	0.44	0.32
17	0	13	79	43	0	135	0.42	3.28	0.46	0.26
18	1	8	81	45	0	135	0.43	3.43	0.48	0.27
19	1	9	77	36	0	123	0.47	4.25	0.55	0.27
20	0	9	79	44	0	132	0.45	4.49	0.54	0.29

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

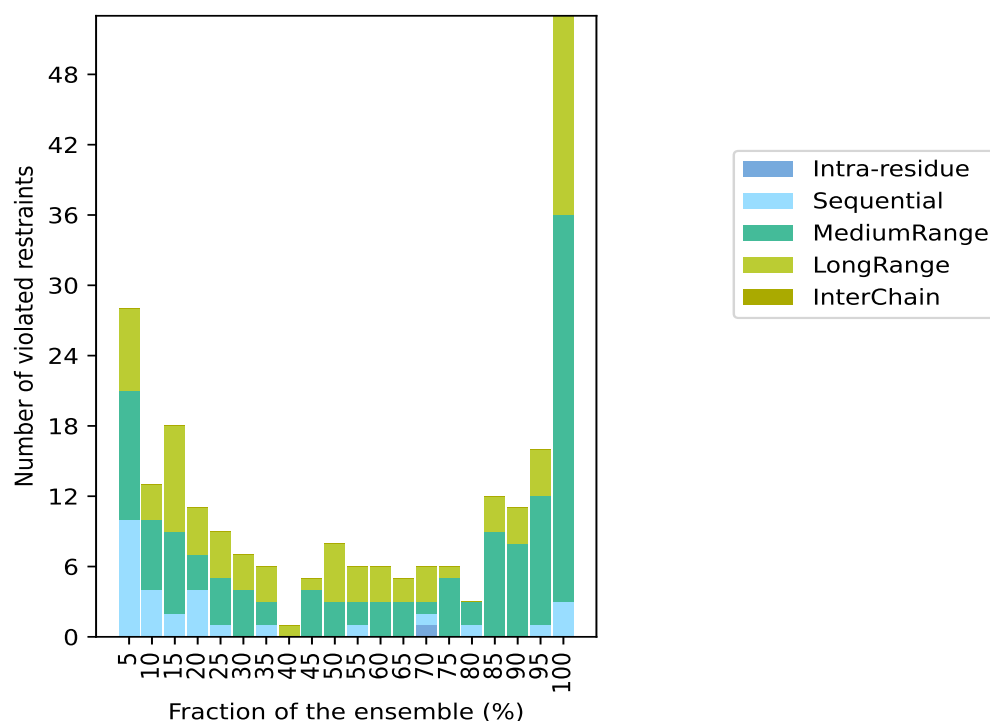
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 291(IR:39, SQ:159, MR:63, LR:30, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	10	11	7	0	28	1	5.0
0	4	6	3	0	13	2	10.0
0	2	7	9	0	18	3	15.0
0	4	3	4	0	11	4	20.0
0	1	4	4	0	9	5	25.0
0	0	4	3	0	7	6	30.0
0	1	2	3	0	6	7	35.0
0	0	0	1	0	1	8	40.0
0	0	4	1	0	5	9	45.0
0	0	3	5	0	8	10	50.0
0	1	2	3	0	6	11	55.0
0	0	3	3	0	6	12	60.0
0	0	3	2	0	5	13	65.0
1	1	1	3	0	6	14	70.0
0	0	5	1	0	6	15	75.0
0	1	2	0	0	3	16	80.0
0	0	9	3	0	12	17	85.0
0	0	8	3	0	11	18	90.0
0	1	11	4	0	16	19	95.0
0	3	33	17	0	53	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

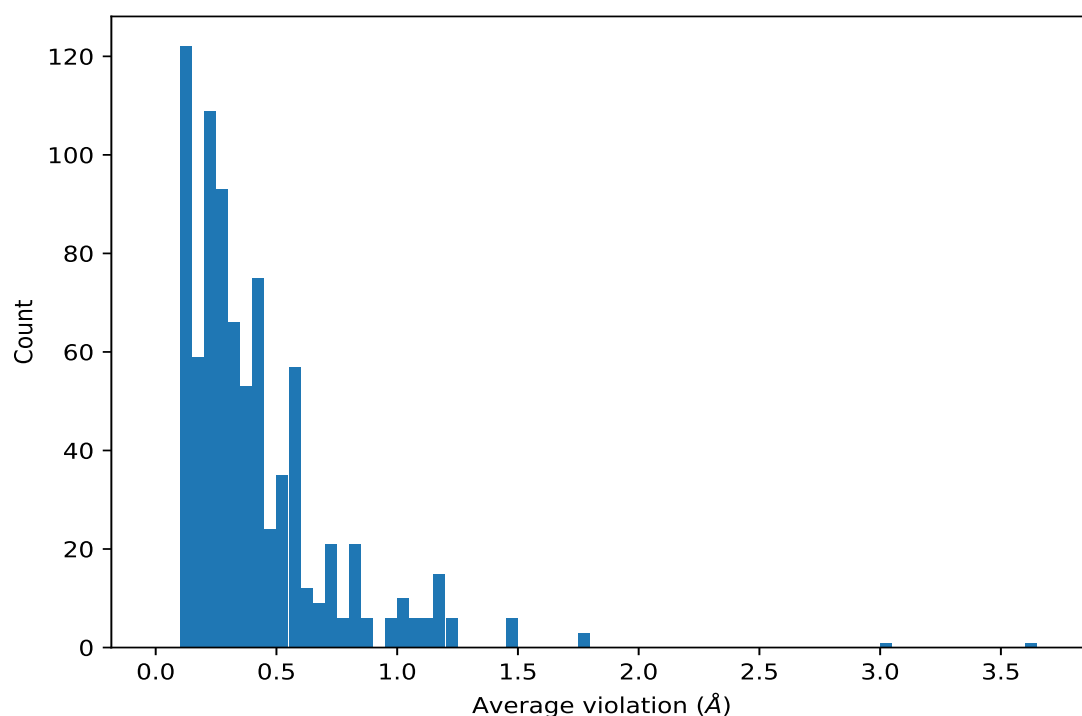
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	20	3.64	0.7	3.49
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	20	3.02	0.46	3.03
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	20	1.77	0.45	1.77
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	20	1.77	0.45	1.77
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	20	1.77	0.45	1.77
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	20	1.46	0.19	1.52
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	20	1.46	0.19	1.52
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	20	1.46	0.19	1.52
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	20	1.46	0.19	1.52
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	20	1.46	0.19	1.52
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	20	1.46	0.19	1.52
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	20	1.24	0.32	1.26
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	20	1.24	0.32	1.26
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	20	1.24	0.32	1.26
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	20	1.24	0.32	1.26
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	20	1.24	0.32	1.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	20	1.24	0.32	1.26
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	20	1.2	0.2	1.2
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	20	1.2	0.2	1.2
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	20	1.2	0.2	1.2
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	20	1.2	0.2	1.2
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	20	1.2	0.2	1.2
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	20	1.2	0.2	1.2
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	20	1.18	0.42	1.44
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	20	1.18	0.42	1.44
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	20	1.18	0.42	1.44
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	20	1.17	0.05	1.17
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	20	1.17	0.05	1.17
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	20	1.17	0.05	1.17
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	20	1.17	0.05	1.17
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	20	1.17	0.05	1.17
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	20	1.17	0.05	1.17
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	20	1.13	0.27	1.16
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	20	1.13	0.27	1.16
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	20	1.13	0.27	1.16
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	20	1.13	0.27	1.16
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	20	1.13	0.27	1.16
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	20	1.13	0.27	1.16
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	20	1.07	0.35	1.19
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	20	1.07	0.35	1.19
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	20	1.07	0.35	1.19
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	20	1.07	0.35	1.19
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	20	1.07	0.35	1.19
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	20	1.07	0.35	1.19
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	20	1.03	0.04	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	20	1.03	0.04	1.04
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	20	1.03	0.03	1.03
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	20	0.87	0.37	0.8
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	20	0.87	0.37	0.8
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	20	0.87	0.37	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	20	0.71	0.08	0.72

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	20	0.71	0.08	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	20	0.71	0.08	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	20	0.71	0.08	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	20	0.71	0.08	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	20	0.71	0.08	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	20	0.6	0.12	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	20	0.6	0.12	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	20	0.6	0.12	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	20	0.6	0.12	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	20	0.6	0.12	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	20	0.6	0.12	0.62
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	20	0.58	0.16	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	20	0.58	0.16	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	20	0.58	0.16	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	20	0.58	0.16	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	20	0.58	0.16	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	20	0.58	0.16	0.65
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	20	0.52	0.07	0.52
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	20	0.52	0.07	0.52
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	20	0.52	0.07	0.52
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	20	0.51	0.18	0.49
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	20	0.49	0.09	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	20	0.49	0.09	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	20	0.49	0.09	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	20	0.49	0.09	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	20	0.49	0.09	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	20	0.49	0.09	0.5
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	20	0.46	0.05	0.44
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	20	0.43	0.05	0.43
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	20	0.43	0.07	0.42
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	20	0.43	0.06	0.44
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	20	0.42	0.05	0.42
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	20	0.41	0.08	0.4
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	20	0.39	0.04	0.4
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	20	0.39	0.05	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	20	0.39	0.05	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	20	0.39	0.05	0.38
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	20	0.38	0.03	0.37
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	20	0.37	0.08	0.34
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	20	0.36	0.04	0.35
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	20	0.35	0.08	0.32
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	20	0.35	0.04	0.34
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	20	0.35	0.05	0.34
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	20	0.34	0.06	0.34
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	20	0.33	0.1	0.34
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	20	0.33	0.05	0.32
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	20	0.33	0.04	0.33
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	20	0.33	0.05	0.32
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	20	0.31	0.03	0.32
(1,238)	1:134:A:MET:H	1:136:A:THR:H	20	0.31	0.06	0.29
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	20	0.28	0.08	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	20	0.28	0.04	0.29
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	20	0.27	0.03	0.26
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	20	0.25	0.06	0.26
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	20	0.24	0.05	0.24
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	20	0.24	0.04	0.22
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	20	0.23	0.04	0.24
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	20	0.23	0.05	0.22
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	20	0.22	0.04	0.22
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	20	0.21	0.06	0.2
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	20	0.2	0.05	0.2
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	20	0.2	0.04	0.19
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	20	0.18	0.04	0.18
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	19	0.81	0.2	0.88
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	19	0.81	0.2	0.88
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	19	0.79	0.27	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	19	0.79	0.27	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	19	0.79	0.27	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	19	0.79	0.27	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	19	0.79	0.27	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	19	0.79	0.27	0.79
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	19	0.71	0.1	0.7
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	19	0.71	0.1	0.7
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	19	0.55	0.18	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	19	0.55	0.18	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	19	0.55	0.18	0.56
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	19	0.45	0.14	0.48
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	19	0.36	0.19	0.29
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	19	0.35	0.15	0.37
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	19	0.27	0.03	0.27
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	19	0.27	0.03	0.27
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	19	0.27	0.03	0.27
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	19	0.27	0.03	0.27
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	19	0.27	0.03	0.27
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	19	0.27	0.03	0.27
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	19	0.25	0.08	0.22
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	19	0.23	0.04	0.22
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	19	0.22	0.07	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	19	0.2	0.05	0.21
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	19	0.2	0.07	0.19
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	19	0.19	0.05	0.18
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	19	0.19	0.05	0.2
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	19	0.18	0.05	0.17
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	18	0.96	0.37	0.97
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	18	0.96	0.37	0.97
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	18	0.96	0.37	0.97
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	18	0.82	0.36	0.98
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	18	0.82	0.36	0.98
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	18	0.82	0.36	0.98
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	18	0.82	0.36	0.98
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	18	0.82	0.36	0.98
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	18	0.82	0.36	0.98
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	18	0.53	0.29	0.42
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	18	0.53	0.29	0.42
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	18	0.53	0.29	0.42
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	18	0.52	0.13	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	18	0.52	0.13	0.54
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	18	0.33	0.1	0.33
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	18	0.27	0.11	0.24
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	18	0.27	0.11	0.24
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	18	0.27	0.11	0.24
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	18	0.26	0.06	0.26
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	18	0.25	0.06	0.23
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	18	0.23	0.04	0.24
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	18	0.22	0.04	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	18	0.22	0.04	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	18	0.22	0.04	0.21
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	18	0.2	0.04	0.19
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	17	0.99	0.25	1.12
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	17	0.99	0.25	1.12
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	17	0.99	0.25	1.12
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	17	0.56	0.32	0.6
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	17	0.56	0.32	0.6
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	17	0.56	0.32	0.6
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	17	0.43	0.16	0.48
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	17	0.26	0.1	0.25
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	17	0.2	0.03	0.2
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	17	0.2	0.04	0.2
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	17	0.2	0.05	0.18
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	17	0.18	0.04	0.17
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	17	0.17	0.04	0.17
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	17	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	17	0.15	0.02	0.15
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	17	0.14	0.02	0.14
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	16	0.27	0.08	0.26
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	16	0.19	0.04	0.18
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	16	0.16	0.05	0.15
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	15	0.46	0.27	0.32
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	15	0.46	0.27	0.32
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	15	0.46	0.27	0.32
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	15	0.46	0.27	0.32
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	15	0.46	0.27	0.32
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	15	0.46	0.27	0.32
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	15	0.26	0.1	0.23
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	15	0.22	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	15	0.22	0.07	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	15	0.22	0.07	0.24
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	15	0.19	0.05	0.19
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	15	0.16	0.03	0.16
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	15	0.14	0.03	0.13
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	14	0.84	0.43	0.76
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	14	0.84	0.43	0.76
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	14	0.84	0.43	0.76
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	14	0.84	0.43	0.76
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	14	0.84	0.43	0.76
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	14	0.84	0.43	0.76
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	14	0.56	0.44	0.45
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	14	0.56	0.44	0.45
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	14	0.56	0.44	0.45
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	14	0.56	0.44	0.45
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	14	0.56	0.44	0.45
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	14	0.56	0.44	0.45
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	14	0.51	0.12	0.53
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	14	0.42	0.17	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	14	0.42	0.17	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	14	0.42	0.17	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	14	0.42	0.17	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	14	0.42	0.17	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	14	0.42	0.17	0.36
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	14	0.25	0.13	0.22
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	14	0.13	0.02	0.12
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	13	0.43	0.19	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	13	0.43	0.19	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	13	0.43	0.19	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	13	0.43	0.19	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	13	0.43	0.19	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	13	0.43	0.19	0.45
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	13	0.25	0.08	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	13	0.25	0.08	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	13	0.25	0.08	0.29
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	13	0.18	0.04	0.18
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	13	0.17	0.03	0.18
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	13	0.15	0.03	0.14
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	12	0.5	0.39	0.34
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	12	0.5	0.39	0.34
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	12	0.5	0.39	0.34
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	12	0.42	0.26	0.33
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	12	0.42	0.26	0.33
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	12	0.42	0.26	0.33
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	12	0.42	0.26	0.33
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	12	0.42	0.26	0.33
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	12	0.42	0.26	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	12	0.32	0.13	0.38
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	12	0.32	0.13	0.38
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	12	0.32	0.13	0.38
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	12	0.22	0.04	0.22
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	12	0.17	0.03	0.17
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	12	0.16	0.04	0.15
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	11	0.61	0.2	0.66
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	11	0.61	0.2	0.66
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	11	0.61	0.2	0.66
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	11	0.41	0.18	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	11	0.41	0.18	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	11	0.41	0.18	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	11	0.41	0.18	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	11	0.41	0.18	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	11	0.41	0.18	0.31
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	11	0.32	0.05	0.3
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	11	0.32	0.05	0.3
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	11	0.32	0.05	0.3
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	11	0.2	0.06	0.2
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	11	0.19	0.05	0.19
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	11	0.19	0.05	0.19
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	11	0.19	0.05	0.19
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	11	0.19	0.05	0.19
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	11	0.19	0.05	0.19
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	11	0.19	0.05	0.19
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	11	0.13	0.02	0.13
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	10	0.86	0.38	0.82
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	10	0.86	0.38	0.82
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	10	0.86	0.38	0.82
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	10	0.47	0.1	0.44
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	10	0.47	0.1	0.44
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	10	0.47	0.1	0.44
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	10	0.47	0.1	0.44
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	10	0.47	0.1	0.44
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	10	0.47	0.1	0.44
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	10	0.41	0.25	0.44
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	10	0.41	0.25	0.44
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	10	0.41	0.25	0.44
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	10	0.41	0.25	0.44
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	10	0.41	0.25	0.44
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	10	0.41	0.25	0.44
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	10	0.21	0.08	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	10	0.21	0.08	0.18
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	10	0.21	0.08	0.18
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	10	0.21	0.08	0.18
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	10	0.21	0.08	0.18
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	10	0.21	0.08	0.18
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	10	0.2	0.05	0.22
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	10	0.2	0.05	0.22
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	10	0.2	0.05	0.22
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	10	0.2	0.05	0.22
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	10	0.2	0.05	0.22
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	10	0.2	0.05	0.22
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	10	0.14	0.02	0.13
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	10	0.14	0.02	0.13
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	10	0.13	0.03	0.12
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	9	0.33	0.13	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	9	0.33	0.13	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	9	0.33	0.13	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	9	0.33	0.13	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	9	0.33	0.13	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	9	0.33	0.13	0.34
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	9	0.16	0.03	0.15
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	9	0.14	0.04	0.13
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	9	0.13	0.02	0.13
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	9	0.13	0.02	0.13
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	8	0.3	0.16	0.24
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	8	0.3	0.16	0.24
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	8	0.3	0.16	0.24
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	7	0.68	0.33	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	7	0.68	0.33	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	7	0.68	0.33	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	7	0.68	0.33	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	7	0.68	0.33	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	7	0.68	0.33	0.73
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	7	0.41	0.14	0.51
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	7	0.41	0.14	0.51
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	7	0.41	0.14	0.51
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	7	0.3	0.09	0.31
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	7	0.3	0.09	0.31
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	7	0.3	0.09	0.31
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	7	0.3	0.09	0.31
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	7	0.3	0.09	0.31
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	7	0.3	0.09	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	7	0.15	0.03	0.14
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	7	0.14	0.05	0.12
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	7	0.11	0.01	0.11
(1,404)	1:12:A:LEU:HD11	1:152:A:TRP:HE1	6	0.25	0.08	0.25
(1,404)	1:12:A:LEU:HD12	1:152:A:TRP:HE1	6	0.25	0.08	0.25
(1,404)	1:12:A:LEU:HD13	1:152:A:TRP:HE1	6	0.25	0.08	0.25
(1,404)	1:12:A:LEU:HD21	1:152:A:TRP:HE1	6	0.25	0.08	0.25
(1,404)	1:12:A:LEU:HD22	1:152:A:TRP:HE1	6	0.25	0.08	0.25
(1,404)	1:12:A:LEU:HD23	1:152:A:TRP:HE1	6	0.25	0.08	0.25
(1,158)	1:102:A:GLY:H	1:104:A:ILE:H	6	0.23	0.08	0.24
(1,394)	1:138:A:LEU:HD11	1:143:A:GLU:H	6	0.22	0.07	0.21
(1,394)	1:138:A:LEU:HD12	1:143:A:GLU:H	6	0.22	0.07	0.21
(1,394)	1:138:A:LEU:HD13	1:143:A:GLU:H	6	0.22	0.07	0.21
(1,505)	1:138:A:LEU:HD11	1:152:A:TRP:HE1	6	0.18	0.04	0.17
(1,505)	1:138:A:LEU:HD12	1:152:A:TRP:HE1	6	0.18	0.04	0.17
(1,505)	1:138:A:LEU:HD13	1:152:A:TRP:HE1	6	0.18	0.04	0.17
(1,505)	1:138:A:LEU:HD21	1:152:A:TRP:HE1	6	0.18	0.04	0.17
(1,505)	1:138:A:LEU:HD22	1:152:A:TRP:HE1	6	0.18	0.04	0.17
(1,505)	1:138:A:LEU:HD23	1:152:A:TRP:HE1	6	0.18	0.04	0.17
(1,152)	1:127:A:VAL:H	1:129:A:ARG:H	6	0.17	0.02	0.16
(1,145)	1:164:A:ALA:H	1:166:A:GLU:H	6	0.13	0.02	0.12
(1,90)	1:8:A:SER:H	1:10:A:ARG:H	6	0.13	0.02	0.12
(1,378)	1:17:A:LEU:HD11	1:113:A:ALA:H	5	0.71	0.41	0.51
(1,378)	1:17:A:LEU:HD12	1:113:A:ALA:H	5	0.71	0.41	0.51
(1,378)	1:17:A:LEU:HD13	1:113:A:ALA:H	5	0.71	0.41	0.51
(1,378)	1:17:A:LEU:HD21	1:113:A:ALA:H	5	0.71	0.41	0.51
(1,378)	1:17:A:LEU:HD22	1:113:A:ALA:H	5	0.71	0.41	0.51
(1,378)	1:17:A:LEU:HD23	1:113:A:ALA:H	5	0.71	0.41	0.51
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG11	5	0.64	0.32	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG12	5	0.64	0.32	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG13	5	0.64	0.32	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG21	5	0.64	0.32	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG22	5	0.64	0.32	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG23	5	0.64	0.32	0.46
(1,448)	1:72:A:LEU:HD11	1:90:A:VAL:H	5	0.36	0.28	0.2
(1,448)	1:72:A:LEU:HD12	1:90:A:VAL:H	5	0.36	0.28	0.2
(1,448)	1:72:A:LEU:HD13	1:90:A:VAL:H	5	0.36	0.28	0.2
(1,448)	1:72:A:LEU:HD21	1:90:A:VAL:H	5	0.36	0.28	0.2
(1,448)	1:72:A:LEU:HD22	1:90:A:VAL:H	5	0.36	0.28	0.2
(1,448)	1:72:A:LEU:HD23	1:90:A:VAL:H	5	0.36	0.28	0.2
(1,338)	1:12:A:LEU:HD21	1:51:A:LYS:H	5	0.32	0.29	0.21
(1,338)	1:12:A:LEU:HD22	1:51:A:LYS:H	5	0.32	0.29	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,338)	1:12:A:LEU:HD23	1:51:A:LYS:H	5	0.32	0.29	0.21
(1,212)	1:99:A:VAL:H	1:102:A:GLY:H	5	0.17	0.05	0.18
(1,149)	1:129:A:ARG:H	1:131:A:ALA:H	5	0.15	0.03	0.16
(1,234)	1:116:A:VAL:H	1:117:A:GLU:H	5	0.14	0.03	0.13
(1,14)	1:92:A:ASN:H	1:94:A:LEU:H	5	0.13	0.01	0.13
(1,68)	1:158:A:LEU:H	1:161:A:ASN:H	5	0.13	0.01	0.12
(1,434)	1:50:A:VAL:HG11	1:152:A:TRP:H	4	0.37	0.2	0.36
(1,434)	1:50:A:VAL:HG12	1:152:A:TRP:H	4	0.37	0.2	0.36
(1,434)	1:50:A:VAL:HG13	1:152:A:TRP:H	4	0.37	0.2	0.36
(1,434)	1:50:A:VAL:HG21	1:152:A:TRP:H	4	0.37	0.2	0.36
(1,434)	1:50:A:VAL:HG22	1:152:A:TRP:H	4	0.37	0.2	0.36
(1,434)	1:50:A:VAL:HG23	1:152:A:TRP:H	4	0.37	0.2	0.36
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD11	4	0.31	0.0	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD12	4	0.31	0.0	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD13	4	0.31	0.0	0.31
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD11	4	0.3	0.12	0.31
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD12	4	0.3	0.12	0.31
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD13	4	0.3	0.12	0.31
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD21	4	0.3	0.12	0.31
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD22	4	0.3	0.12	0.31
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD23	4	0.3	0.12	0.31
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD11	4	0.29	0.11	0.27
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD12	4	0.29	0.11	0.27
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD13	4	0.29	0.11	0.27
(1,79)	1:27:A:SER:H	1:30:A:GLN:H	4	0.22	0.11	0.18
(1,150)	1:126:A:LEU:H	1:129:A:ARG:H	4	0.16	0.05	0.16
(1,177)	1:156:A:VAL:H	1:159:A:TYR:H	4	0.16	0.05	0.14
(1,5)	1:65:A:TYR:H	1:66:A:ARG:H	4	0.14	0.02	0.14
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG11	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG12	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG13	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG21	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG22	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG23	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG11	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG12	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG13	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG21	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG22	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG23	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG11	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG12	4	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG13	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG21	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG22	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG23	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG11	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG12	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG13	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG21	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG22	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG23	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG11	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG12	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG13	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG21	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG22	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG23	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG11	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG12	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG13	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG21	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG22	4	0.13	0.02	0.13
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG23	4	0.13	0.02	0.13
(1,231)	1:66:A:ARG:H	1:67:A:ARG:H	4	0.13	0.03	0.13
(1,268)	1:162:A:ASN:H	1:163:A:ALA:H	4	0.11	0.01	0.11
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD21	3	0.61	0.11	0.64
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD22	3	0.61	0.11	0.64
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD23	3	0.61	0.11	0.64
(1,454)	1:72:A:LEU:HD11	1:111:A:GLY:H	3	0.52	0.31	0.48
(1,454)	1:72:A:LEU:HD12	1:111:A:GLY:H	3	0.52	0.31	0.48
(1,454)	1:72:A:LEU:HD13	1:111:A:GLY:H	3	0.52	0.31	0.48
(1,454)	1:72:A:LEU:HD21	1:111:A:GLY:H	3	0.52	0.31	0.48
(1,454)	1:72:A:LEU:HD22	1:111:A:GLY:H	3	0.52	0.31	0.48
(1,454)	1:72:A:LEU:HD23	1:111:A:GLY:H	3	0.52	0.31	0.48
(1,362)	1:72:A:LEU:HD21	1:110:A:PHE:H	3	0.51	0.29	0.45
(1,362)	1:72:A:LEU:HD22	1:110:A:PHE:H	3	0.51	0.29	0.45
(1,362)	1:72:A:LEU:HD23	1:110:A:PHE:H	3	0.51	0.29	0.45
(1,246)	1:22:A:SER:H	1:26:A:TYR:H	3	0.49	0.25	0.66
(1,282)	1:12:A:LEU:HD11	1:51:A:LYS:H	3	0.48	0.22	0.37
(1,282)	1:12:A:LEU:HD12	1:51:A:LYS:H	3	0.48	0.22	0.37
(1,282)	1:12:A:LEU:HD13	1:51:A:LYS:H	3	0.48	0.22	0.37
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG11	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG12	3	0.44	0.06	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG13	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG21	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG22	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG23	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG11	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG12	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG13	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG21	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG22	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG23	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG11	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG12	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG13	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG21	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG22	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG23	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG11	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG12	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG13	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG21	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG22	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG23	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG11	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG12	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG13	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG21	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG22	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG23	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG11	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG12	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG13	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG21	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG22	3	0.44	0.06	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG23	3	0.44	0.06	0.48
(1,377)	1:17:A:LEU:HD11	1:111:A:GLY:H	3	0.28	0.14	0.23
(1,377)	1:17:A:LEU:HD12	1:111:A:GLY:H	3	0.28	0.14	0.23
(1,377)	1:17:A:LEU:HD13	1:111:A:GLY:H	3	0.28	0.14	0.23
(1,377)	1:17:A:LEU:HD21	1:111:A:GLY:H	3	0.28	0.14	0.23
(1,377)	1:17:A:LEU:HD22	1:111:A:GLY:H	3	0.28	0.14	0.23
(1,377)	1:17:A:LEU:HD23	1:111:A:GLY:H	3	0.28	0.14	0.23
(1,105)	1:33:A:ASP:H	1:35:A:GLU:H	3	0.18	0.03	0.17
(2,6)	1:78:A:ILE:HD11	1:128:A:SER:H	3	0.17	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,6)	1:78:A:ILE:HD12	1:128:A:SER:H	3	0.17	0.02	0.18
(2,6)	1:78:A:ILE:HD13	1:128:A:SER:H	3	0.17	0.02	0.18
(1,511)	1:158:A:LEU:HD11	1:160:A:GLY:H	3	0.16	0.05	0.13
(1,511)	1:158:A:LEU:HD12	1:160:A:GLY:H	3	0.16	0.05	0.13
(1,511)	1:158:A:LEU:HD13	1:160:A:GLY:H	3	0.16	0.05	0.13
(1,511)	1:158:A:LEU:HD21	1:160:A:GLY:H	3	0.16	0.05	0.13
(1,511)	1:158:A:LEU:HD22	1:160:A:GLY:H	3	0.16	0.05	0.13
(1,511)	1:158:A:LEU:HD23	1:160:A:GLY:H	3	0.16	0.05	0.13
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD11	3	0.16	0.05	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD12	3	0.16	0.05	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD13	3	0.16	0.05	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD21	3	0.16	0.05	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD22	3	0.16	0.05	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD23	3	0.16	0.05	0.14
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD21	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD22	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD23	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD21	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD22	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD23	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD21	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD22	3	0.15	0.04	0.13
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD23	3	0.15	0.04	0.13
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD21	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD22	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD23	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD21	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD22	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD23	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD21	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD22	3	0.15	0.03	0.16
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD23	3	0.15	0.03	0.16
(1,263)	1:68:A:ALA:H	1:70:A:SER:H	3	0.14	0.03	0.13
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG11	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG12	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG13	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG21	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG22	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG23	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG11	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG12	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG13	3	0.14	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG21	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG22	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG23	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG11	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG12	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG13	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG21	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG22	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG23	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG11	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG12	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG13	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG21	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG22	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG23	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG11	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG12	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG13	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG21	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG22	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG23	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG11	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG12	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG13	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG21	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG22	3	0.14	0.04	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG23	3	0.14	0.04	0.14
(1,21)	1:43:A:GLU:H	1:44:A:GLY:H	3	0.14	0.04	0.11
(1,91)	1:10:A:ARG:H	1:12:A:LEU:H	3	0.14	0.02	0.13
(1,189)	1:69:A:PHE:H	1:72:A:LEU:H	3	0.13	0.02	0.12
(1,355)	1:99:A:VAL:HG11	1:101:A:TRP:HE1	2	0.65	0.03	0.65
(1,355)	1:99:A:VAL:HG12	1:101:A:TRP:HE1	2	0.65	0.03	0.65
(1,355)	1:99:A:VAL:HG13	1:101:A:TRP:HE1	2	0.65	0.03	0.65
(1,421)	1:21:A:LEU:HD11	1:26:A:TYR:H	2	0.53	0.04	0.53
(1,421)	1:21:A:LEU:HD12	1:26:A:TYR:H	2	0.53	0.04	0.53
(1,421)	1:21:A:LEU:HD13	1:26:A:TYR:H	2	0.53	0.04	0.53
(1,421)	1:21:A:LEU:HD21	1:26:A:TYR:H	2	0.53	0.04	0.53
(1,421)	1:21:A:LEU:HD22	1:26:A:TYR:H	2	0.53	0.04	0.53
(1,421)	1:21:A:LEU:HD23	1:26:A:TYR:H	2	0.53	0.04	0.53
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG11	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG12	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG13	2	0.34	0.05	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG21	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG22	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG23	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG11	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG12	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG13	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG21	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG22	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG23	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG11	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG12	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG13	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG21	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG22	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG23	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG11	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG12	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG13	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG21	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG22	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG23	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG11	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG12	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG13	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG21	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG22	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG23	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG11	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG12	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG13	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG21	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG22	2	0.34	0.05	0.34
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG23	2	0.34	0.05	0.34
(1,221)	1:125:A:VAL:H	1:127:A:VAL:H	2	0.29	0.1	0.29
(1,466)	1:94:A:LEU:HD11	1:106:A:ALA:H	2	0.26	0.14	0.26
(1,466)	1:94:A:LEU:HD12	1:106:A:ALA:H	2	0.26	0.14	0.26
(1,466)	1:94:A:LEU:HD13	1:106:A:ALA:H	2	0.26	0.14	0.26
(1,466)	1:94:A:LEU:HD21	1:106:A:ALA:H	2	0.26	0.14	0.26
(1,466)	1:94:A:LEU:HD22	1:106:A:ALA:H	2	0.26	0.14	0.26
(1,466)	1:94:A:LEU:HD23	1:106:A:ALA:H	2	0.26	0.14	0.26
(1,214)	1:26:A:TYR:H	1:27:A:SER:H	2	0.23	0.01	0.23
(1,72)	1:88:A:GLU:H	1:91:A:VAL:H	2	0.18	0.02	0.18

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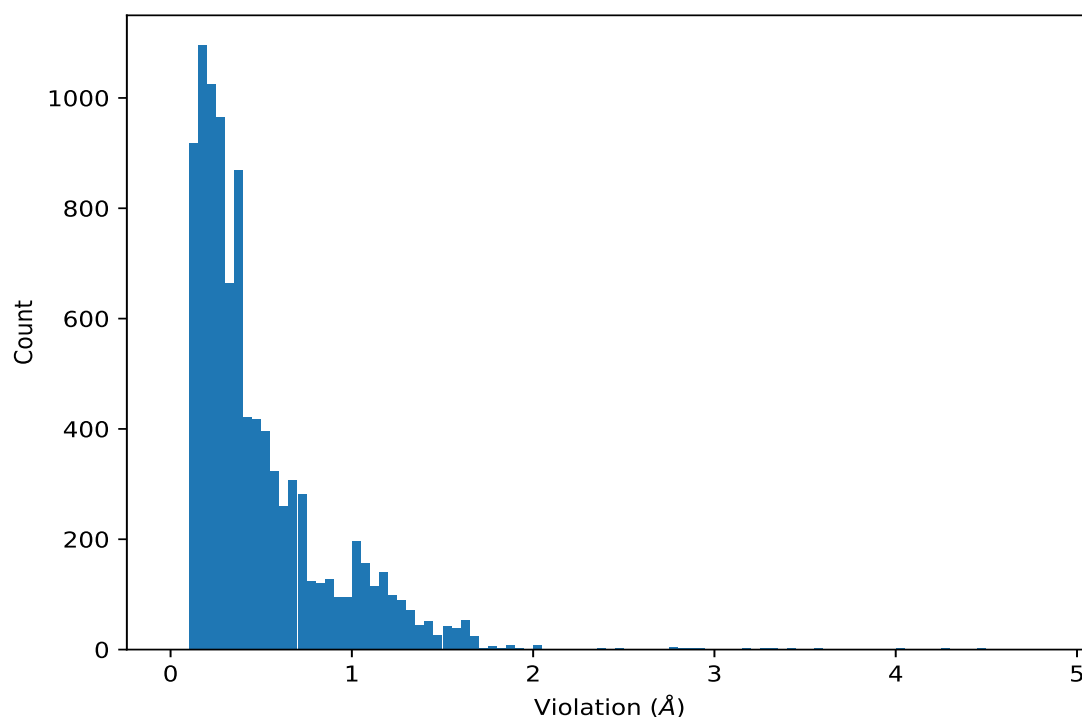
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,170)	1:40:A:GLU:H	1:41:A:ALA:H	2	0.18	0.06	0.18
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD11	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD12	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD13	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD11	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD12	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD13	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD11	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD12	2	0.18	0.0	0.18
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD13	2	0.18	0.0	0.18
(1,17)	1:106:A:ALA:H	1:109:A:SER:H	2	0.15	0.02	0.15
(1,60)	1:13:A:VAL:H	1:16:A:PHE:H	2	0.15	0.04	0.15
(1,35)	1:131:A:ALA:H	1:133:A:TRP:H	2	0.13	0.01	0.13
(1,191)	1:101:A:TRP:H	1:102:A:GLY:H	2	0.12	0.0	0.12

¹Number of violated models, ²Standard 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)
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	1	4.81
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	9	4.6
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	14	4.49
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	20	4.49
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	7	4.39
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	8	4.26
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	19	4.25
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	4	4.04
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	13	4.03
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	15	3.76
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	12	3.55
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	2	3.55
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	15	3.46
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	18	3.43
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	2	3.4
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	14	3.38
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	1	3.34
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	10	3.32
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	17	3.28
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	3	3.25
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	5	3.24
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	6	3.19
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	6	3.15
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	19	3.14
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	3	3.01
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	13	2.93
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	20	2.91
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	16	2.9
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	4	2.89
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	18	2.88
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	11	2.82
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	17	2.82
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	8	2.81
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	3	2.78
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	3	2.78
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	3	2.78
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	5	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	11	2.65
(2,3)	1:24:A:LYS:H	1:30:A:GLN:H	12	2.62
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	10	2.54
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	13	2.45
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	13	2.45
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	13	2.45
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	7	2.42
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	14	2.39
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	14	2.39
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	14	2.39
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	9	2.23
(2,5)	1:142:A:LEU:H	1:152:A:TRP:HE1	16	2.11
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	17	2.04
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	17	2.04
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	17	2.04
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	1	2.02
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	1	2.02
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	1	2.02
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	2	2.0
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	2	2.0
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	2	2.0
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	20	1.94
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	20	1.94
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	20	1.94
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	18	1.86
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	18	1.86
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	18	1.86
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	16	1.85
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	16	1.85
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	16	1.85
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	16	1.85
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	16	1.85
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	16	1.85
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	12	1.83
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	12	1.83
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	12	1.83
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	15	1.78
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	15	1.78
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	15	1.78
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	19	1.76
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	19	1.76
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	19	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	5	1.71
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	5	1.71
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	5	1.71
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	11	1.69
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	11	1.69
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	11	1.69
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	3	1.69
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	3	1.69
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	3	1.69
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	7	1.67
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	7	1.67
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	7	1.67
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	7	1.67
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	7	1.67
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	7	1.67
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	3	1.66
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	3	1.66
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	3	1.66
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	3	1.66
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	3	1.66
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	3	1.66
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	20	1.65
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	20	1.65
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	20	1.65
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	20	1.65
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	20	1.65
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	20	1.65
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	18	1.64
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	18	1.64
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	18	1.64
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	18	1.64
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	18	1.64
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	18	1.64
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	11	1.63
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	11	1.63
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	11	1.63
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	11	1.63
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	11	1.63
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	11	1.63
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	19	1.63
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	19	1.63
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	19	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	19	1.63
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	19	1.63
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	19	1.63
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	2	1.63
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	2	1.63
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	2	1.63
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	5	1.62
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	5	1.62
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	5	1.62
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	5	1.62
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	5	1.62
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	5	1.62
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	8	1.62
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	8	1.62
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	8	1.62
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	8	1.62
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	8	1.62
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	8	1.62
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	16	1.62
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	16	1.62
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	16	1.62
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	16	1.62
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	16	1.62
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	16	1.62
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	7	1.62
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	7	1.62
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	7	1.62
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	10	1.61
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	10	1.61
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	10	1.61
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	10	1.61
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	10	1.61
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	10	1.61
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	18	1.6
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	18	1.6
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	18	1.6
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	18	1.6
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	18	1.6
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	18	1.6
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	11	1.58
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	11	1.58
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	11	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	11	1.58
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	11	1.58
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	11	1.58
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	5	1.58
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	5	1.58
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	5	1.58
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	20	1.57
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	20	1.57
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	20	1.57
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	4	1.57
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	4	1.57
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	4	1.57
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	4	1.56
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	4	1.56
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	4	1.56
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	4	1.56
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	4	1.56
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	4	1.56
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	14	1.56
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	14	1.56
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	14	1.56
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	15	1.56
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	15	1.56
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	15	1.56
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	4	1.55
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	4	1.55
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	4	1.55
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	4	1.55
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	4	1.55
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	4	1.55
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	11	1.55
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	11	1.55
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	11	1.55
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	11	1.55
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	11	1.55
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	11	1.55
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	12	1.53
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	12	1.53
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	12	1.53
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	12	1.53
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	12	1.53
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	12	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	10	1.53
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	10	1.53
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	10	1.53
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	20	1.52
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	20	1.52
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	20	1.52
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	20	1.52
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	20	1.52
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	20	1.52
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	13	1.52
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	13	1.52
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	13	1.52
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	13	1.52
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	13	1.52
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	13	1.52
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	18	1.52
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	18	1.52
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	18	1.52
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	8	1.51
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	8	1.51
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	8	1.51
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	8	1.51
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	8	1.51
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	8	1.51
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	6	1.51
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	6	1.51
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	6	1.51
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	12	1.51
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	12	1.51
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	12	1.51
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	12	1.51
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	12	1.51
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	12	1.51
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	1	1.5
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	1	1.5
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	1	1.5
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	10	1.49
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	10	1.49
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	10	1.49
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	10	1.49
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	10	1.49
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	10	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	7	1.49
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	7	1.49
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	7	1.49
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	18	1.48
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	18	1.48
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	18	1.48
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	18	1.48
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	18	1.48
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	18	1.48
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	8	1.46
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	8	1.46
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	8	1.46
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	16	1.46
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	16	1.46
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	16	1.46
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	17	1.45
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	17	1.45
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	17	1.45
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	17	1.45
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	17	1.45
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	17	1.45
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	5	1.44
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	5	1.44
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	5	1.44
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	5	1.44
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	5	1.44
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	5	1.44
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	6	1.44
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	6	1.44
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	6	1.44
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	6	1.44
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	6	1.44
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	6	1.44
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	14	1.44
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	14	1.44
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	14	1.44
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	14	1.44
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	14	1.44
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	14	1.44
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	20	1.43
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	20	1.43
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	20	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	20	1.43
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	20	1.43
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	20	1.43
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	2	1.43
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	2	1.43
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	2	1.43
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	6	1.43
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	6	1.43
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	6	1.43
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	10	1.42
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	10	1.42
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	10	1.42
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	10	1.42
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	10	1.42
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	10	1.42
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	17	1.4
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	17	1.4
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	17	1.4
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	17	1.4
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	17	1.4
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	17	1.4
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	20	1.4
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	20	1.4
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	20	1.4
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	20	1.4
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	20	1.4
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	20	1.4
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	20	1.4
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	20	1.4
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	20	1.4
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	7	1.39
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	7	1.39
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	7	1.39
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	7	1.39
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	7	1.39
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	7	1.39
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	7	1.38
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	7	1.38
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	7	1.38
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	7	1.38
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	7	1.38
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	7	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	1	1.38
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	1	1.38
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	1	1.38
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	1	1.38
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	1	1.38
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	1	1.38
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	19	1.38
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	19	1.38
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	19	1.38
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	9	1.36
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	9	1.36
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	9	1.36
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	9	1.36
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	9	1.36
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	9	1.36
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	15	1.36
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	15	1.36
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	15	1.36
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	15	1.36
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	15	1.36
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	15	1.36
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	12	1.36
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	12	1.36
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	12	1.36
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	12	1.36
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	12	1.36
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	12	1.36
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	19	1.36
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	19	1.36
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	19	1.36
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	5	1.35
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	5	1.35
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	5	1.35
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	19	1.33
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	19	1.33
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	19	1.33
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	19	1.33
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	19	1.33
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	19	1.33
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	8	1.33
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	8	1.33
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	8	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	8	1.33
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	8	1.33
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	8	1.33
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	1	1.33
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	1	1.33
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	1	1.33
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	1	1.33
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	1	1.33
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	1	1.33
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	9	1.33
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	9	1.33
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	9	1.33
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	9	1.33
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	9	1.33
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	9	1.33
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	13	1.32
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	13	1.32
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	13	1.32
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	13	1.32
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	13	1.32
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	13	1.32
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	12	1.32
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	12	1.32
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	12	1.32
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	12	1.32
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	12	1.32
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	12	1.32
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	8	1.32
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	8	1.32
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	8	1.32
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	13	1.32
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	13	1.32
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	13	1.32
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	7	1.32
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	7	1.32
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	7	1.32
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	17	1.31
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	17	1.31
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	17	1.31
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	17	1.31
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	17	1.31
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	17	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	13	1.31
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	13	1.31
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	13	1.31
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	10	1.3
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	10	1.3
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	10	1.3
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	10	1.3
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	10	1.3
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	10	1.3
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	14	1.3
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	14	1.3
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	14	1.3
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	14	1.3
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	14	1.3
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	14	1.3
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	9	1.3
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	9	1.3
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	9	1.3
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	9	1.3
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	9	1.3
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	9	1.3
(1,378)	1:17:A:LEU:HD11	1:113:A:ALA:H	12	1.29
(1,378)	1:17:A:LEU:HD12	1:113:A:ALA:H	12	1.29
(1,378)	1:17:A:LEU:HD13	1:113:A:ALA:H	12	1.29
(1,378)	1:17:A:LEU:HD21	1:113:A:ALA:H	12	1.29
(1,378)	1:17:A:LEU:HD22	1:113:A:ALA:H	12	1.29
(1,378)	1:17:A:LEU:HD23	1:113:A:ALA:H	12	1.29
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	14	1.29
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	14	1.29
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	14	1.29
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	14	1.29
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	14	1.29
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	14	1.29
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	4	1.28
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	4	1.28
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	4	1.28
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	4	1.28
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	4	1.28
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	4	1.28
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	7	1.28
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	7	1.28
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	7	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	1	1.27
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	1	1.27
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	1	1.27
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	1	1.27
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	1	1.27
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	1	1.27
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	12	1.27
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	12	1.27
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	12	1.27
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	12	1.27
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	12	1.27
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	12	1.27
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	9	1.27
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	9	1.27
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	9	1.27
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	9	1.27
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	9	1.27
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	9	1.27
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	17	1.27
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	17	1.27
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	17	1.27
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	17	1.27
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	17	1.27
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	17	1.27
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	10	1.27
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	10	1.27
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	10	1.27
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	19	1.27
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	19	1.27
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	19	1.27
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	19	1.27
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	19	1.27
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	19	1.27
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	7	1.27
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	7	1.27
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	7	1.27
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	7	1.27
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	7	1.27
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	7	1.27
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	6	1.26
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	6	1.26
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	6	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	6	1.26
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	6	1.26
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	6	1.26
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	19	1.26
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	19	1.26
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	19	1.26
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	19	1.26
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	19	1.26
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	19	1.26
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	3	1.25
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	3	1.25
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	3	1.25
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	3	1.25
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	3	1.25
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	3	1.25
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	15	1.25
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	15	1.25
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	15	1.25
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	15	1.25
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	15	1.25
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	15	1.25
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	7	1.25
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	7	1.25
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	7	1.25
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	7	1.25
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	7	1.25
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	7	1.25
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	2	1.23
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	2	1.23
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	2	1.23
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	2	1.23
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	2	1.23
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	2	1.23
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	2	1.23
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	2	1.23
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	2	1.23
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	2	1.23
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	2	1.23
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	2	1.23
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	18	1.22
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	18	1.22
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	18	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	18	1.22
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	18	1.22
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	18	1.22
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	19	1.22
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	19	1.22
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	19	1.22
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	19	1.22
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	19	1.22
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	19	1.22
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	2	1.22
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	2	1.22
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	2	1.22
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	2	1.22
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	2	1.22
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	2	1.22
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	17	1.22
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	17	1.22
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	17	1.22
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	16	1.22
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	16	1.22
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	16	1.22
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	16	1.22
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	16	1.22
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	16	1.22
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	16	1.22
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	16	1.22
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	16	1.22
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	16	1.22
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	16	1.22
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	16	1.22
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	17	1.22
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	17	1.22
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	17	1.22
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	8	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	8	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	8	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	8	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	8	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	8	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	16	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	16	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	16	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	16	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	16	1.21
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	16	1.21
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	14	1.2
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	14	1.2
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	14	1.2
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	14	1.2
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	14	1.2
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	14	1.2
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	18	1.2
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	18	1.2
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	18	1.2
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	18	1.2
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	18	1.2
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	18	1.2
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	8	1.2
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	8	1.2
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	8	1.2
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	8	1.2
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	8	1.2
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	8	1.2
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	9	1.2
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	9	1.2
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	9	1.2
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	9	1.2
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	9	1.2
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	9	1.2
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	3	1.2
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	3	1.2
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	3	1.2
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	3	1.2
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	3	1.2
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	3	1.2
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	19	1.2
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	19	1.2
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	19	1.2
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG11	16	1.2
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG12	16	1.2
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG13	16	1.2
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG21	16	1.2
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG22	16	1.2
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG23	16	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	7	1.19
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	7	1.19
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	7	1.19
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	7	1.19
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	7	1.19
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	7	1.19
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	12	1.19
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	12	1.19
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	12	1.19
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	9	1.19
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	9	1.19
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	9	1.19
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	15	1.19
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	15	1.19
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	15	1.19
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	1	1.18
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	1	1.18
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	1	1.18
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	1	1.18
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	1	1.18
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	1	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	6	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	6	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	6	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	6	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	6	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	6	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	10	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	10	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	10	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	10	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	10	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	10	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	13	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	13	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	13	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	13	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	13	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	13	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	15	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	15	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	15	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	15	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	15	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	15	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	20	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	20	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	20	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	20	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	20	1.18
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	20	1.18
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	20	1.18
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	20	1.18
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	20	1.18
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	20	1.18
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	20	1.18
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	20	1.18
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	14	1.18
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	14	1.18
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	14	1.18
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	5	1.17
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	5	1.17
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	5	1.17
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	5	1.17
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	5	1.17
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	5	1.17
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	13	1.17
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	13	1.17
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	13	1.17
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	13	1.17
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	13	1.17
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	13	1.17
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	2	1.16
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	2	1.16
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	2	1.16
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	2	1.16
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	2	1.16
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	2	1.16
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	13	1.16
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	13	1.16
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	13	1.16
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	13	1.16
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	13	1.16
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	13	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	4	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	4	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	4	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	4	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	4	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	4	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	12	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	12	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	12	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	12	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	12	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	12	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	14	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	14	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	14	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	14	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	14	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	14	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	19	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	19	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	19	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	19	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	19	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	19	1.16
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	4	1.16
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	4	1.16
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	4	1.16
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	5	1.16
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	5	1.16
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	5	1.16
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	7	1.16
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	7	1.16
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	7	1.16
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	10	1.16
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	10	1.16
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	10	1.16
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	10	1.16
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	10	1.16
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	10	1.16
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	2	1.15
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	2	1.15
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	2	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	2	1.15
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	2	1.15
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	2	1.15
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	16	1.15
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	16	1.15
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	16	1.15
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	16	1.15
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	16	1.15
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	16	1.15
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	16	1.15
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	16	1.15
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	16	1.15
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	16	1.15
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	16	1.15
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	16	1.15
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	6	1.14
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	6	1.14
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	6	1.14
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	6	1.14
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	6	1.14
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	6	1.14
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	3	1.14
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	3	1.14
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	3	1.14
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	3	1.14
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	3	1.14
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	3	1.14
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	4	1.14
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	4	1.14
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	4	1.14
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	4	1.14
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	4	1.14
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	4	1.14
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	3	1.14
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	3	1.14
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	3	1.14
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	1	1.13
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	1	1.13
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	1	1.13
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	1	1.13
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	1	1.13
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	1	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	18	1.13
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	18	1.13
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	18	1.13
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	18	1.13
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	18	1.13
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	18	1.13
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	11	1.13
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	11	1.13
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	11	1.13
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	4	1.12
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	4	1.12
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	4	1.12
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	4	1.12
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	4	1.12
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	4	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	9	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	9	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	9	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	9	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	9	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	9	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	11	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	11	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	11	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	11	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	11	1.12
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	11	1.12
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	1	1.12
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	1	1.12
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	1	1.12
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	1	1.12
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	1	1.12
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	1	1.12
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	4	1.12
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	4	1.12
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	4	1.12
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	4	1.12
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	4	1.12
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	4	1.12
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	2	1.12
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	2	1.12
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	2	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	2	1.12
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	2	1.12
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	2	1.12
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	9	1.12
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	9	1.12
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	9	1.12
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	12	1.12
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	12	1.12
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	12	1.12
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	2	1.11
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	2	1.11
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	2	1.11
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	2	1.11
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	2	1.11
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	2	1.11
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	7	1.11
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	7	1.11
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	7	1.11
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	7	1.11
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	7	1.11
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	7	1.11
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	6	1.11
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	6	1.11
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	6	1.11
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	1	1.1
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	1	1.1
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	1	1.1
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	1	1.1
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	1	1.1
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	1	1.1
(1,378)	1:17:A:LEU:HD11	1:113:A:ALA:H	3	1.1
(1,378)	1:17:A:LEU:HD12	1:113:A:ALA:H	3	1.1
(1,378)	1:17:A:LEU:HD13	1:113:A:ALA:H	3	1.1
(1,378)	1:17:A:LEU:HD21	1:113:A:ALA:H	3	1.1
(1,378)	1:17:A:LEU:HD22	1:113:A:ALA:H	3	1.1
(1,378)	1:17:A:LEU:HD23	1:113:A:ALA:H	3	1.1
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	8	1.1
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	8	1.1
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	8	1.1
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	8	1.1
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	8	1.1
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	8	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	8	1.1
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	8	1.1
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	8	1.1
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	6	1.1
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	19	1.09
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	19	1.09
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	19	1.09
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	19	1.09
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	19	1.09
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	19	1.09
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	3	1.09
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	3	1.09
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	3	1.09
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	3	1.09
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	3	1.09
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	3	1.09
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	3	1.09
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	3	1.09
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	3	1.09
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	15	1.09
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	15	1.09
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	15	1.09
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	15	1.09
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	15	1.09
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	15	1.09
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	15	1.09
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	15	1.09
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	15	1.09
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	2	1.09
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	2	1.09
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	2	1.09
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	8	1.08
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	8	1.08
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	8	1.08
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	8	1.08
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	8	1.08
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	8	1.08
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	16	1.08
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	16	1.08
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	16	1.08
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	16	1.08
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	16	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	16	1.08
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	5	1.08
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	5	1.08
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	5	1.08
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	5	1.08
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	5	1.08
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	5	1.08
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	5	1.08
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	5	1.08
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	5	1.08
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	10	1.08
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	10	1.08
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	10	1.08
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	14	1.08
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	5	1.07
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	5	1.07
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	5	1.07
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	5	1.07
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	5	1.07
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	5	1.07
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	6	1.07
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	6	1.07
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	6	1.07
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	6	1.07
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	6	1.07
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	6	1.07
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	6	1.07
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	6	1.07
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	6	1.07
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	6	1.07
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	6	1.07
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	6	1.07
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	6	1.07
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	6	1.07
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	6	1.07
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	5	1.07
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	5	1.07
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	5	1.07
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	5	1.07
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	3	1.06
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	3	1.06
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	3	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	3	1.06
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	3	1.06
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	3	1.06
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	11	1.06
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	11	1.06
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	11	1.06
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	11	1.06
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	11	1.06
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	11	1.06
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	2	1.06
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	2	1.06
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	2	1.06
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	2	1.06
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	2	1.06
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	2	1.06
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	2	1.06
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	2	1.06
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	2	1.06
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	10	1.06
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	10	1.06
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	10	1.06
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	10	1.06
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	10	1.06
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	10	1.06
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	10	1.06
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	10	1.06
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	10	1.06
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	6	1.06
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	6	1.06
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	6	1.06
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	6	1.06
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	6	1.06
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	6	1.06
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	16	1.06
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	15	1.05
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	15	1.05
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	15	1.05
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	15	1.05
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	15	1.05
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	15	1.05
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	11	1.05
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	11	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	11	1.05
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	11	1.05
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	11	1.05
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	11	1.05
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	19	1.05
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	19	1.05
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	19	1.05
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	19	1.05
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	19	1.05
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	19	1.05
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG11	5	1.05
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG12	5	1.05
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG13	5	1.05
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG21	5	1.05
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG22	5	1.05
(1,440)	1:54:A:LEU:H	1:156:A:VAL:HG23	5	1.05
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	5	1.05
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	5	1.05
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	5	1.05
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	5	1.05
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	5	1.05
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	5	1.05
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	9	1.05
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	9	1.05
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	9	1.05
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	1	1.05
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	1	1.05
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	1	1.05
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	1	1.05
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	1	1.05
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	1	1.05
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	1	1.05
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	1	1.05
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	1	1.05
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	3	1.05
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	19	1.04
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	19	1.04
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	19	1.04
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	19	1.04
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	19	1.04
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	19	1.04
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	16	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	16	1.04
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	16	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	3	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	3	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	3	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	3	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	3	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	3	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	3	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	3	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	3	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	4	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	4	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	4	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	4	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	4	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	4	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	4	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	4	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	4	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	20	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	20	1.04
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	20	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	20	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	20	1.04
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	20	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	20	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	20	1.04
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	20	1.04
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	16	1.04
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	16	1.04
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	16	1.04
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	2	1.04
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	7	1.04
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	10	1.04
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	12	1.04
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	13	1.03
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	13	1.03
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	13	1.03
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	13	1.03
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	13	1.03
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	13	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	11	1.03
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	11	1.03
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	11	1.03
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	11	1.03
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	11	1.03
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	11	1.03
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	11	1.03
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	11	1.03
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	11	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	7	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	7	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	7	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	7	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	7	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	7	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	7	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	7	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	7	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	13	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	13	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	13	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	13	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	13	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	13	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	13	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	13	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	13	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	18	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	18	1.03
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	18	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	18	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	18	1.03
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	18	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	18	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	18	1.03
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	18	1.03
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	1	1.03
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	9	1.03
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	11	1.03
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	13	1.02
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	13	1.02
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	13	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	13	1.02
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	13	1.02
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	13	1.02
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	20	1.02
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	20	1.02
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	20	1.02
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	20	1.02
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	20	1.02
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	20	1.02
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	9	1.02
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	9	1.02
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	9	1.02
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	9	1.02
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	9	1.02
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	9	1.02
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	9	1.02
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	9	1.02
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	9	1.02
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	17	1.02
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	17	1.02
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	17	1.02
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	12	1.02
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	12	1.02
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	12	1.02
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	12	1.02
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	12	1.02
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	12	1.02
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	4	1.02
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	8	1.02
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	13	1.02
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	18	1.02
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	19	1.02
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	14	1.01
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	14	1.01
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	14	1.01
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	14	1.01
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	14	1.01
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	14	1.01
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	16	1.01
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	16	1.01
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	16	1.01
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	16	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	16	1.01
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	16	1.01
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	4	1.01
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	4	1.01
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	4	1.01
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	4	1.01
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	4	1.01
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	4	1.01
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	4	1.01
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	4	1.01
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	4	1.01
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	4	1.01
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	4	1.01
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	4	1.01
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	11	1.01
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	11	1.01
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	11	1.01
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	11	1.01
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	11	1.01
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	11	1.01
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	11	1.01
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	11	1.01
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	11	1.01
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	14	1.01
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	14	1.01
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	14	1.01
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	14	1.01
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	14	1.01
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	14	1.01
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	14	1.01
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	14	1.01
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	14	1.01
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	13	1.01
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	13	1.01
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	13	1.01
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	4	1.0
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	4	1.0
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	4	1.0
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	4	1.0
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	4	1.0
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	4	1.0
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	1	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	1	1.0
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	1	1.0
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	1	1.0
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	1	1.0
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	1	1.0
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	1	1.0
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	1	1.0
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	1	1.0
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	16	1.0
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	16	1.0
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	16	1.0
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	16	1.0
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	16	1.0
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	16	1.0
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	16	1.0
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	16	1.0
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	16	1.0
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	14	1.0
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	14	1.0
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	14	1.0
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	20	1.0
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	9	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	9	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	9	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	9	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	9	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	9	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	9	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	9	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	9	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	13	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	13	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	13	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	13	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	13	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	13	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	13	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	13	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	13	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	19	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	19	0.99
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	19	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	19	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	19	0.99
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	19	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	19	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	19	0.99
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	19	0.99
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	17	0.99
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	17	0.99
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	17	0.99
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	17	0.99
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	17	0.99
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	17	0.99
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	17	0.99
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	17	0.99
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	17	0.99
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	19	0.99
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	19	0.99
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	19	0.99
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	19	0.99
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	19	0.99
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	19	0.99
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	19	0.99
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	19	0.99
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	19	0.99
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	10	0.98
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	10	0.98
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	10	0.98
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	10	0.98
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	10	0.98
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	10	0.98
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	11	0.98
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	11	0.98
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	11	0.98
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	15	0.98
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	13	0.97
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	13	0.97
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	13	0.97
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	13	0.97
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	13	0.97
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	13	0.97
(1,102)	1:139:A:ASN:H	1:141:A:HIS:H	17	0.97
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	17	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	17	0.96
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	17	0.96
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	18	0.96
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	18	0.96
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	18	0.96
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	17	0.95
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	17	0.95
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	17	0.95
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	17	0.95
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	17	0.95
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	17	0.95
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	2	0.95
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	2	0.95
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	2	0.95
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	2	0.95
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	2	0.95
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	2	0.95
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	14	0.95
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	14	0.95
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	14	0.95
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	14	0.95
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	14	0.95
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	14	0.95
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	14	0.95
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	14	0.95
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	14	0.95
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	7	0.95
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	7	0.95
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	7	0.95
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	7	0.95
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	7	0.95
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	7	0.95
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	2	0.94
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	2	0.94
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	2	0.94
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	2	0.94
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	2	0.94
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	2	0.94
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	7	0.94
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	7	0.94
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	7	0.94
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	7	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	7	0.94
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	7	0.94
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	3	0.94
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	3	0.94
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	3	0.94
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	3	0.94
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	3	0.94
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	3	0.94
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD11	12	0.94
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD12	12	0.94
(1,348)	1:138:A:LEU:HD21	1:146:A:ILE:HD13	12	0.94
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD11	12	0.94
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD12	12	0.94
(1,348)	1:138:A:LEU:HD22	1:146:A:ILE:HD13	12	0.94
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD11	12	0.94
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD12	12	0.94
(1,348)	1:138:A:LEU:HD23	1:146:A:ILE:HD13	12	0.94
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	3	0.94
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	3	0.94
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	3	0.94
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	1	0.94
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	1	0.94
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	1	0.94
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	1	0.94
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	1	0.94
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	1	0.94
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	9	0.94
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	9	0.94
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	9	0.94
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	9	0.94
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	9	0.94
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	9	0.94
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	20	0.93
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	20	0.93
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	20	0.93
(1,347)	1:146:A:ILE:HD11	1:152:A:TRP:HE1	10	0.93
(1,347)	1:146:A:ILE:HD12	1:152:A:TRP:HE1	10	0.93
(1,347)	1:146:A:ILE:HD13	1:152:A:TRP:HE1	10	0.93
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	12	0.93
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	12	0.93
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	12	0.93
(1,411)	1:13:A:VAL:HG11	1:131:A:ALA:H	15	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:13:A:VAL:HG12	1:131:A:ALA:H	15	0.92
(1,411)	1:13:A:VAL:HG13	1:131:A:ALA:H	15	0.92
(1,411)	1:13:A:VAL:HG21	1:131:A:ALA:H	15	0.92
(1,411)	1:13:A:VAL:HG22	1:131:A:ALA:H	15	0.92
(1,411)	1:13:A:VAL:HG23	1:131:A:ALA:H	15	0.92
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	16	0.92
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	16	0.92
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	16	0.92
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	11	0.92
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	11	0.92
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	11	0.92
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	16	0.92
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	16	0.92
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	16	0.92
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	6	0.92
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	6	0.92
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	6	0.92
(1,454)	1:72:A:LEU:HD11	1:111:A:GLY:H	16	0.91
(1,454)	1:72:A:LEU:HD12	1:111:A:GLY:H	16	0.91
(1,454)	1:72:A:LEU:HD13	1:111:A:GLY:H	16	0.91
(1,454)	1:72:A:LEU:HD21	1:111:A:GLY:H	16	0.91
(1,454)	1:72:A:LEU:HD22	1:111:A:GLY:H	16	0.91
(1,454)	1:72:A:LEU:HD23	1:111:A:GLY:H	16	0.91
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	18	0.91
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	18	0.91
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	18	0.91
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	18	0.91
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	18	0.91
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	18	0.91
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	18	0.91
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	18	0.91
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	18	0.91
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	3	0.91
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	3	0.91
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	3	0.91
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	10	0.91
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	10	0.91
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	10	0.91
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	17	0.91
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	17	0.91
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	17	0.91
(1,362)	1:72:A:LEU:HD21	1:110:A:PHE:H	11	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:72:A:LEU:HD22	1:110:A:PHE:H	11	0.9
(1,362)	1:72:A:LEU:HD23	1:110:A:PHE:H	11	0.9
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	9	0.89
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	9	0.89
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	9	0.89
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	12	0.89
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	12	0.89
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	12	0.89
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	6	0.89
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	6	0.89
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	6	0.89
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	6	0.89
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	6	0.89
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	6	0.89
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	6	0.89
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	6	0.89
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	6	0.89
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	6	0.89
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	6	0.89
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	6	0.89
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	6	0.89
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	6	0.89
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	6	0.89
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	6	0.89
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	6	0.89
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	6	0.89
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	6	0.89
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	6	0.89
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	6	0.89
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	6	0.89
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	6	0.89
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	6	0.89
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	6	0.89
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	6	0.89
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	6	0.89
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	6	0.89
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	6	0.89
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	6	0.89
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	6	0.89
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	6	0.89
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	6	0.89
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	6	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	6	0.89
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	6	0.89
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	3	0.89
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	3	0.89
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	3	0.89
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	3	0.89
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	3	0.89
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	3	0.89
(1,448)	1:72:A:LEU:HD11	1:90:A:VAL:H	11	0.89
(1,448)	1:72:A:LEU:HD12	1:90:A:VAL:H	11	0.89
(1,448)	1:72:A:LEU:HD13	1:90:A:VAL:H	11	0.89
(1,448)	1:72:A:LEU:HD21	1:90:A:VAL:H	11	0.89
(1,448)	1:72:A:LEU:HD22	1:90:A:VAL:H	11	0.89
(1,448)	1:72:A:LEU:HD23	1:90:A:VAL:H	11	0.89
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	15	0.89
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	15	0.89
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	15	0.89
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	15	0.89
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	15	0.89
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	15	0.89
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	12	0.89
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	12	0.89
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	12	0.89
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	12	0.89
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	12	0.89
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	12	0.89
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	15	0.89
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	15	0.89
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	15	0.89
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	15	0.89
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	15	0.89
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	15	0.89
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	15	0.89
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	15	0.89
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	15	0.89
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	12	0.89
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	12	0.89
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	12	0.89
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	16	0.88
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	16	0.88
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	16	0.88
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	16	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	16	0.88
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	16	0.88
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	16	0.88
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	16	0.88
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	16	0.88
(1,338)	1:12:A:LEU:HD21	1:51:A:LYS:H	2	0.88
(1,338)	1:12:A:LEU:HD22	1:51:A:LYS:H	2	0.88
(1,338)	1:12:A:LEU:HD23	1:51:A:LYS:H	2	0.88
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	17	0.88
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	17	0.88
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	17	0.88
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	8	0.87
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	8	0.87
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	8	0.87
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	11	0.87
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	13	0.86
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	13	0.86
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	13	0.86
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	13	0.86
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	13	0.86
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	13	0.86
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	13	0.86
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	13	0.86
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	13	0.86
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	15	0.86
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	15	0.86
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	15	0.86
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	15	0.86
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	15	0.86
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	15	0.86
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	15	0.86
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	15	0.86
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	15	0.86
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	18	0.85
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	18	0.85
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	18	0.85
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	18	0.85
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	18	0.85
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	18	0.85
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	8	0.85
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	8	0.85
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	8	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	8	0.85
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	8	0.85
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	8	0.85
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	12	0.84
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	12	0.84
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	12	0.84
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	12	0.84
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	12	0.84
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	12	0.84
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	12	0.84
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	12	0.84
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	12	0.84
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	12	0.84
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	12	0.84
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	12	0.84
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	12	0.84
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	12	0.84
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	12	0.84
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	12	0.84
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	12	0.84
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	12	0.84
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	12	0.84
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	12	0.84
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	12	0.84
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	12	0.84
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	12	0.84
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	12	0.84
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	12	0.84
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	12	0.84
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	12	0.84
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	12	0.84
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	12	0.84
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	12	0.84
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	12	0.84
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	12	0.84
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	12	0.84
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	12	0.84
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	12	0.84
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	12	0.84
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	12	0.84
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	12	0.84
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	12	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	12	0.84
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	12	0.84
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	12	0.84
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	11	0.84
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	11	0.84
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	11	0.84
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	11	0.84
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	11	0.84
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	11	0.84
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	8	0.84
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	8	0.84
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	8	0.84
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	9	0.84
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	9	0.84
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	9	0.84
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	3	0.83
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	3	0.83
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	3	0.83
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	3	0.83
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	3	0.83
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	3	0.83
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	8	0.83
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	8	0.83
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	8	0.83
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	8	0.83
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	8	0.83
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	8	0.83
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	8	0.83
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	8	0.83
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	8	0.83
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	6	0.82
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	6	0.82
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	6	0.82
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	6	0.82
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	6	0.82
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	6	0.82
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	14	0.82
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	14	0.82
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	14	0.82
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	14	0.82
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	14	0.82
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	14	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	14	0.82
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	14	0.82
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	14	0.82
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	8	0.81
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	8	0.81
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	8	0.81
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	8	0.81
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	8	0.81
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	8	0.81
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	8	0.81
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	8	0.81
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	8	0.81
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	4	0.81
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	4	0.81
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	4	0.81
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	5	0.81
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	5	0.81
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	5	0.81
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	5	0.81
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	5	0.81
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	5	0.81
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	7	0.81
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	7	0.81
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	7	0.81
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	5	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	5	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	5	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	5	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	5	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	5	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	12	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	12	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	12	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	12	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	12	0.8
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	12	0.8
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	9	0.8
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	9	0.8
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	9	0.8
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	18	0.79
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	18	0.79
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	18	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	18	0.79
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	18	0.79
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	18	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	7	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	7	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	7	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	7	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	7	0.79
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	7	0.79
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	15	0.79
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	15	0.79
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	15	0.79
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	15	0.79
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	15	0.79
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	15	0.79
(1,282)	1:12:A:LEU:HD11	1:51:A:LYS:H	7	0.79
(1,282)	1:12:A:LEU:HD12	1:51:A:LYS:H	7	0.79
(1,282)	1:12:A:LEU:HD13	1:51:A:LYS:H	7	0.79
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	13	0.79
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	17	0.78
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	17	0.78
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	17	0.78
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	17	0.78
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	17	0.78
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	17	0.78
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	17	0.78
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	17	0.78
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	17	0.78
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	15	0.78
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	15	0.78
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	15	0.78
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	11	0.78
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	11	0.78
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	11	0.78
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	11	0.78
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	11	0.78
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	11	0.78
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	11	0.78
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	11	0.78
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	11	0.78
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG11	9	0.78
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG12	9	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG13	9	0.78
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG21	9	0.78
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG22	9	0.78
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG23	9	0.78
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	6	0.78
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	6	0.78
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	6	0.78
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	20	0.77
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	20	0.77
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	20	0.77
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	20	0.77
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	20	0.77
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	20	0.77
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	9	0.77
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	9	0.77
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	9	0.77
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	6	0.76
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	6	0.76
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	6	0.76
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	6	0.76
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	6	0.76
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	6	0.76
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	1	0.76
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	1	0.76
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	1	0.76
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	1	0.76
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	1	0.76
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	1	0.76
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	18	0.76
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	18	0.76
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	18	0.76
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	18	0.76
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	18	0.76
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	18	0.76
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	2	0.76
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	2	0.76
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	2	0.76
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	2	0.76
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	2	0.76
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	2	0.76
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	2	0.76
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	2	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	2	0.76
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	6	0.76
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	6	0.76
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	6	0.76
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	6	0.76
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	6	0.76
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	6	0.76
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	6	0.76
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	6	0.76
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	6	0.76
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	1	0.76
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	1	0.76
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	1	0.76
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	6	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	6	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	6	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	6	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	6	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	6	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	15	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	15	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	15	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	15	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	15	0.75
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	15	0.75
(1,412)	1:13:A:VAL:HG11	1:132:A:ALA:H	15	0.75
(1,412)	1:13:A:VAL:HG12	1:132:A:ALA:H	15	0.75
(1,412)	1:13:A:VAL:HG13	1:132:A:ALA:H	15	0.75
(1,412)	1:13:A:VAL:HG21	1:132:A:ALA:H	15	0.75
(1,412)	1:13:A:VAL:HG22	1:132:A:ALA:H	15	0.75
(1,412)	1:13:A:VAL:HG23	1:132:A:ALA:H	15	0.75
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	12	0.75
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	12	0.75
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	12	0.75
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	12	0.75
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	12	0.75
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	12	0.75
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	14	0.74
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	14	0.74
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	14	0.74
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	14	0.74
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	14	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	14	0.74
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	14	0.74
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	14	0.74
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	14	0.74
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	14	0.74
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	14	0.74
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	14	0.74
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	14	0.74
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	14	0.74
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	14	0.74
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	14	0.74
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	14	0.74
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	14	0.74
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	14	0.74
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	14	0.74
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	14	0.74
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	14	0.74
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	14	0.74
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	14	0.74
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	14	0.74
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	14	0.74
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	14	0.74
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	14	0.74
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	14	0.74
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	14	0.74
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	14	0.74
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	14	0.74
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	14	0.74
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	14	0.74
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	14	0.74
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	14	0.74
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	17	0.74
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	17	0.74
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	17	0.74
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	17	0.74
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	17	0.74
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	17	0.74
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	18	0.74
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	18	0.74
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	18	0.74
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	18	0.74
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	18	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	18	0.74
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	20	0.74
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	20	0.74
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	20	0.74
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	20	0.74
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	20	0.74
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	20	0.74
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	20	0.74
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	20	0.74
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	20	0.74
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	14	0.74
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	14	0.74
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	14	0.74
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	14	0.74
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	14	0.74
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	14	0.74
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	14	0.74
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	14	0.74
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	14	0.74
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	4	0.74
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	4	0.73
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	4	0.73
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	4	0.73
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	4	0.73
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	4	0.73
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	4	0.73
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	9	0.73
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	9	0.73
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	9	0.73
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	9	0.73
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	9	0.73
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	9	0.73
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	16	0.73
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	16	0.73
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	16	0.73
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	16	0.73
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	16	0.73
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	16	0.73
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	16	0.73
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	16	0.73
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	16	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	9	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	9	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	9	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	9	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	9	0.73
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	9	0.73
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD21	3	0.73
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD22	3	0.73
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD23	3	0.73
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	15	0.73
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	19	0.72
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	19	0.72
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	19	0.72
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	19	0.72
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	19	0.72
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	19	0.72
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	11	0.72
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	11	0.72
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	11	0.72
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	11	0.72
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	11	0.72
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	11	0.72
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	11	0.72
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	11	0.72
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	11	0.72
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	11	0.72
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	11	0.72
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	11	0.72
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	11	0.72
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	11	0.72
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	11	0.72
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	11	0.72
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	11	0.72
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	11	0.72
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	11	0.72
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	11	0.72
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	11	0.72
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	11	0.72
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	11	0.72
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	11	0.72
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	11	0.72
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	11	0.72
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	11	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	11	0.72
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	11	0.72
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	11	0.72
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	11	0.72
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	11	0.72
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	11	0.72
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	11	0.72
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	11	0.72
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	11	0.72
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	16	0.72
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	16	0.72
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	16	0.72
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	16	0.72
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	16	0.72
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	16	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	13	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	13	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	13	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	13	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	13	0.72
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	13	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	17	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	17	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	17	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	17	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	17	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	17	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	20	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	20	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	20	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	20	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	20	0.72
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	20	0.72
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	17	0.72
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	17	0.72
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	17	0.72
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	17	0.72
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	17	0.72
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	17	0.72
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	20	0.72
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	20	0.72
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	20	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	18	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	18	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	18	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	18	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	18	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	18	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	19	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	19	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	19	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	19	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	19	0.71
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	19	0.71
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	18	0.71
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	18	0.71
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	18	0.71
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	18	0.71
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	18	0.71
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	18	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	2	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	2	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	2	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	2	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	2	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	2	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	3	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	3	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	3	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	3	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	3	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	3	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	7	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	7	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	7	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	7	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	7	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	7	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	8	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	8	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	8	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	8	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	8	0.71
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	8	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	16	0.71
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	16	0.71
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	16	0.71
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	16	0.71
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	16	0.71
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	16	0.71
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	5	0.71
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	5	0.71
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	5	0.71
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	5	0.71
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	5	0.71
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	5	0.71
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	5	0.71
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	5	0.71
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	5	0.71
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	12	0.71
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	12	0.71
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	12	0.71
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	12	0.71
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	12	0.71
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	12	0.71
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	12	0.71
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	12	0.71
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	12	0.71
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	18	0.71
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	18	0.71
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	18	0.71
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	7	0.7
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	2	0.7
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	2	0.7
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	2	0.7
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	2	0.7
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	2	0.7
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	2	0.7
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	16	0.7
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	16	0.7
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	16	0.7
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	16	0.7
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	16	0.7
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	16	0.7
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	11	0.7
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	11	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	11	0.7
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	11	0.7
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	11	0.7
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	11	0.7
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	17	0.7
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	17	0.7
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	17	0.7
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	8	0.7
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	8	0.7
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	8	0.7
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	3	0.7
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	3	0.7
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	3	0.7
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	7	0.7
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	7	0.7
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	7	0.7
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	7	0.7
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	7	0.7
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	7	0.7
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	7	0.7
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	7	0.7
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	7	0.7
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	2	0.7
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	2	0.7
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	2	0.7
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	1	0.69
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	1	0.69
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	1	0.69
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	1	0.69
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	1	0.69
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	1	0.69
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	10	0.69
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	10	0.69
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	10	0.69
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	10	0.69
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	10	0.69
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	10	0.69
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	1	0.69
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	1	0.69
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	1	0.69
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	1	0.69
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	1	0.69
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	4	0.69
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	4	0.69
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	4	0.69
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	4	0.69
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	4	0.69
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	4	0.69
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	7	0.69
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	7	0.69
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	7	0.69
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	7	0.69
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	7	0.69
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	7	0.69
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	15	0.69
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	15	0.69
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	15	0.69
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	15	0.69
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	15	0.69
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	15	0.69
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	4	0.69
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	4	0.69
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	4	0.69
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	4	0.69
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	4	0.69
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	4	0.69
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	4	0.69
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	4	0.69
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	4	0.69
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	9	0.69
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	3	0.68
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	3	0.68
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	3	0.68
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	3	0.68
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	3	0.68
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	3	0.68
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	14	0.68
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	14	0.68
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	14	0.68
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	19	0.68
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	19	0.68
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	19	0.68
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	19	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	19	0.68
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	19	0.68
(1,355)	1:99:A:VAL:HG11	1:101:A:TRP:HE1	1	0.68
(1,355)	1:99:A:VAL:HG12	1:101:A:TRP:HE1	1	0.68
(1,355)	1:99:A:VAL:HG13	1:101:A:TRP:HE1	1	0.68
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	8	0.68
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	8	0.68
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	8	0.68
(1,246)	1:22:A:SER:H	1:26:A:TYR:H	15	0.68
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	20	0.68
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	8	0.68
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	13	0.67
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	13	0.67
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	13	0.67
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	13	0.67
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	13	0.67
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	13	0.67
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	18	0.67
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	18	0.67
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	18	0.67
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	20	0.67
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	19	0.67
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	19	0.67
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	19	0.67
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	19	0.67
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	19	0.67
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	19	0.67
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	19	0.67
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	19	0.67
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	19	0.67
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	19	0.67
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	19	0.67
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	19	0.67
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	19	0.67
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	19	0.67
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	19	0.67
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	19	0.67
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	19	0.67
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	19	0.67
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	19	0.67
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	19	0.67
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	19	0.67
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	19	0.67
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	19	0.67
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	19	0.67
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	19	0.67
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	19	0.67
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	19	0.67
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	19	0.67
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	19	0.67
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	19	0.67
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	19	0.67
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	19	0.67
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	19	0.67
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	19	0.67
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	19	0.67
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	20	0.67
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	20	0.67
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	20	0.67
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	20	0.67
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	20	0.67
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	20	0.67
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	11	0.67
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	11	0.67
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	11	0.67
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	11	0.67
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	11	0.67
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	11	0.67
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	18	0.67
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	18	0.67
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	18	0.67
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	5	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	5	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	5	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	5	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	5	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	5	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	16	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	16	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	16	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	16	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	16	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	16	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	10	0.66
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	10	0.66
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	10	0.66
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	11	0.66
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	11	0.66
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	11	0.66
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	13	0.66
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	13	0.66
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	13	0.66
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	18	0.66
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	18	0.66
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	18	0.66
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	18	0.66
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	18	0.66
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	18	0.66
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	18	0.66
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	18	0.66
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	18	0.66
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	18	0.66
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	18	0.66
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	18	0.66
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	18	0.66
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	18	0.66
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	18	0.66
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	18	0.66
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	18	0.66
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	18	0.66
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	18	0.66
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	18	0.66
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	18	0.66
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	18	0.66
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	18	0.66
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	18	0.66
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	18	0.66
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	18	0.66
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	18	0.66
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	18	0.66
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	18	0.66
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	18	0.66
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	18	0.66
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	18	0.66
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	18	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	18	0.66
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	18	0.66
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	18	0.66
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	10	0.66
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	10	0.66
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	10	0.66
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	10	0.66
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	10	0.66
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	10	0.66
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	9	0.66
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	9	0.66
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	9	0.66
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	9	0.66
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	9	0.66
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	9	0.66
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	16	0.66
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	16	0.66
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	16	0.66
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	16	0.66
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	16	0.66
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	16	0.66
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	16	0.66
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	16	0.66
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	16	0.66
(1,246)	1:22:A:SER:H	1:26:A:TYR:H	8	0.66
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	4	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	4	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	4	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	4	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	4	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	4	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	7	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	7	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	7	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	7	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	7	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	7	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	14	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	14	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	14	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	14	0.65
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	14	0.65
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	3	0.65
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	3	0.65
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	3	0.65
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	3	0.65
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	3	0.65
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	3	0.65
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	3	0.65
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	3	0.65
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	3	0.65
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	3	0.65
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	3	0.65
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	3	0.65
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	3	0.65
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	3	0.65
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	3	0.65
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	3	0.65
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	3	0.65
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	3	0.65
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	3	0.65
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	3	0.65
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	3	0.65
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	3	0.65
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	3	0.65
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	3	0.65
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	3	0.65
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	3	0.65
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	3	0.65
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	3	0.65
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	3	0.65
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	3	0.65
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	3	0.65
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	3	0.65
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	3	0.65
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	3	0.65
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	3	0.65
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	3	0.65
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	19	0.65
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	19	0.65
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	19	0.65
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	19	0.65
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	19	0.65
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	15	0.65
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	15	0.65
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	15	0.65
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	15	0.65
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	15	0.65
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	15	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	2	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	2	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	2	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	2	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	2	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	2	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	7	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	7	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	7	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	7	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	7	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	7	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	16	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	16	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	16	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	16	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	16	0.65
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	16	0.65
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	1	0.65
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	1	0.65
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	1	0.65
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	1	0.65
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	1	0.65
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	1	0.65
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	1	0.65
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	1	0.65
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	1	0.65
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	8	0.65
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	8	0.65
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	8	0.65
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	2	0.65
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	6	0.64
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	6	0.64
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	6	0.64
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	6	0.64
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	6	0.64
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	5	0.64
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	5	0.64
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	5	0.64
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	4	0.64
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	4	0.64
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	4	0.64
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD21	9	0.64
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD22	9	0.64
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD23	9	0.64
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	15	0.64
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	9	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	9	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	9	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	9	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	9	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	9	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	11	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	11	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	11	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	11	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	11	0.63
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	11	0.63
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	20	0.63
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	20	0.63
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	20	0.63
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	5	0.63
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	15	0.63
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	15	0.63
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	15	0.63
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	15	0.63
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	15	0.63
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	15	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	14	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	14	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	14	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	14	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	14	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	14	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	18	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	18	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	18	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	18	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	18	0.63
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	18	0.63
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	12	0.63
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	12	0.63
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	12	0.63
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	12	0.63
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	12	0.63
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	12	0.63
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	12	0.63
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	12	0.63
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	12	0.63
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	20	0.63
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	20	0.63
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	20	0.63
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	20	0.63
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	20	0.63
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	20	0.63
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	20	0.63
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	20	0.63
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	20	0.63
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	20	0.63
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	20	0.63
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	20	0.63
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	20	0.63
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	20	0.63
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	20	0.63
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	3	0.63
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	3	0.63
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	3	0.63
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	3	0.63
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	3	0.63
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	3	0.63
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	15	0.63
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	15	0.63
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	15	0.63
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	13	0.62
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	13	0.62
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	13	0.62
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	16	0.62
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	16	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	16	0.62
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	16	0.62
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	16	0.62
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	16	0.62
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	16	0.62
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	16	0.62
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	16	0.62
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	16	0.62
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	16	0.62
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	16	0.62
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	16	0.62
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	16	0.62
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	16	0.62
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	16	0.62
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	16	0.62
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	16	0.62
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	16	0.62
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	16	0.62
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	16	0.62
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	16	0.62
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	16	0.62
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	16	0.62
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	16	0.62
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	16	0.62
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	16	0.62
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	16	0.62
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	16	0.62
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	16	0.62
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	16	0.62
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	16	0.62
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	16	0.62
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	16	0.62
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	16	0.62
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	16	0.62
(1,434)	1:50:A:VAL:HG11	1:152:A:TRP:H	7	0.62
(1,434)	1:50:A:VAL:HG12	1:152:A:TRP:H	7	0.62
(1,434)	1:50:A:VAL:HG13	1:152:A:TRP:H	7	0.62
(1,434)	1:50:A:VAL:HG21	1:152:A:TRP:H	7	0.62
(1,434)	1:50:A:VAL:HG22	1:152:A:TRP:H	7	0.62
(1,434)	1:50:A:VAL:HG23	1:152:A:TRP:H	7	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	3	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	3	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	3	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	3	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	3	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	3	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	5	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	5	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	5	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	5	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	5	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	5	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	19	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	19	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	19	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	19	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	19	0.62
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	19	0.62
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	9	0.62
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	9	0.62
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	9	0.62
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	9	0.62
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	9	0.62
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	9	0.62
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	9	0.62
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	9	0.62
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	9	0.62
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	17	0.62
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	17	0.62
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	17	0.62
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	17	0.62
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	17	0.62
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	17	0.62
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	17	0.62
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	17	0.62
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	17	0.62
(1,355)	1:99:A:VAL:HG11	1:101:A:TRP:HE1	16	0.62
(1,355)	1:99:A:VAL:HG12	1:101:A:TRP:HE1	16	0.62
(1,355)	1:99:A:VAL:HG13	1:101:A:TRP:HE1	16	0.62
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	14	0.62
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	12	0.61
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	12	0.61
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	12	0.61
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	12	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	12	0.61
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	12	0.61
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	12	0.61
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	12	0.61
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	12	0.61
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	12	0.61
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	12	0.61
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	12	0.61
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	17	0.61
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	17	0.61
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	17	0.61
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	17	0.61
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	17	0.61
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	17	0.61
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	12	0.61
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	12	0.61
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	12	0.61
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	3	0.61
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	3	0.61
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	3	0.61
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	3	0.61
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	3	0.61
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	3	0.61
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	3	0.61
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	3	0.61
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	3	0.61
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	13	0.61
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	13	0.61
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	13	0.61
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	15	0.61
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	15	0.61
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	15	0.61
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	15	0.61
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	15	0.61
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	15	0.61
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	4	0.61
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	15	0.61
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	10	0.61
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	4	0.61
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	10	0.61
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	15	0.61
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	15	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	15	0.6
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	15	0.6
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	15	0.6
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	15	0.6
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	15	0.6
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	2	0.6
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	2	0.6
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	2	0.6
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	17	0.6
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	17	0.6
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	17	0.6
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	15	0.6
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	15	0.6
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	15	0.6
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	15	0.6
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	15	0.6
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	15	0.6
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	8	0.6
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	8	0.6
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	8	0.6
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	8	0.6
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	8	0.6
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	8	0.6
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	1	0.6
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	1	0.6
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	1	0.6
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	1	0.6
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	1	0.6
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	1	0.6
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	6	0.6
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	6	0.6
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	6	0.6
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	6	0.6
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	6	0.6
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	6	0.6
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	6	0.6
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	6	0.6
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	6	0.6
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	13	0.6
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	13	0.6
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	13	0.6
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	13	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	13	0.6
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	13	0.6
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	17	0.6
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	17	0.6
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	17	0.6
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	13	0.59
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	13	0.59
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	13	0.59
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	13	0.59
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	13	0.59
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	13	0.59
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	19	0.59
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	19	0.59
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	19	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	10	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	10	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	10	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	10	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	10	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	10	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	12	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	12	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	12	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	12	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	12	0.59
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	12	0.59
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	11	0.59
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	11	0.59
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	11	0.59
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	10	0.59
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	10	0.59
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	10	0.59
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	10	0.59
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	10	0.59
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	10	0.59
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	10	0.59
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	10	0.59
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	10	0.59
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	19	0.59
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	19	0.59
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	19	0.59
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	19	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	19	0.59
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	19	0.59
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	19	0.59
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	19	0.59
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	19	0.59
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	4	0.59
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	4	0.59
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	4	0.59
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	18	0.59
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	18	0.59
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	18	0.59
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	18	0.59
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	18	0.59
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	18	0.59
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	2	0.59
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	17	0.58
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	17	0.58
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	17	0.58
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	17	0.58
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	17	0.58
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	17	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	4	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	4	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	4	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	4	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	4	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	4	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	5	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	5	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	5	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	5	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	5	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	5	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	10	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	10	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	10	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	10	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	10	0.58
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	10	0.58
(1,421)	1:21:A:LEU:HD11	1:26:A:TYR:H	13	0.58
(1,421)	1:21:A:LEU:HD12	1:26:A:TYR:H	13	0.58
(1,421)	1:21:A:LEU:HD13	1:26:A:TYR:H	13	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:21:A:LEU:HD21	1:26:A:TYR:H	13	0.58
(1,421)	1:21:A:LEU:HD22	1:26:A:TYR:H	13	0.58
(1,421)	1:21:A:LEU:HD23	1:26:A:TYR:H	13	0.58
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	6	0.58
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	6	0.58
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	6	0.58
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	6	0.58
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	6	0.58
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	6	0.58
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	12	0.58
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	12	0.58
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	12	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	2	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	2	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	2	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	2	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	2	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	2	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	2	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	2	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	2	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	9	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	9	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	9	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	9	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	9	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	9	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	9	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	9	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	9	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	13	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	13	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	13	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	13	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	13	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	13	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	13	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	13	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	13	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	15	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	15	0.58
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	15	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	15	0.58
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	15	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	15	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	15	0.58
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	15	0.58
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD11	18	0.58
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD12	18	0.58
(1,356)	1:99:A:VAL:HG11	1:104:A:ILE:HD13	18	0.58
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD11	18	0.58
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD12	18	0.58
(1,356)	1:99:A:VAL:HG12	1:104:A:ILE:HD13	18	0.58
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD11	18	0.58
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD12	18	0.58
(1,356)	1:99:A:VAL:HG13	1:104:A:ILE:HD13	18	0.58
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	10	0.57
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	10	0.57
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	10	0.57
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	10	0.57
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	10	0.57
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	10	0.57
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	8	0.57
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	8	0.57
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	8	0.57
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	11	0.57
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	5	0.57
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	5	0.57
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	5	0.57
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	5	0.57
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	5	0.57
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	5	0.57
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	5	0.57
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	5	0.57
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	5	0.57
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	5	0.57
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	5	0.57
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	5	0.57
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	5	0.57
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	5	0.57
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	5	0.57
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	5	0.57
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	5	0.57
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	5	0.57
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	5	0.57
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	5	0.57
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	5	0.57
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	5	0.57
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	5	0.57
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	5	0.57
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	5	0.57
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	5	0.57
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	5	0.57
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	5	0.57
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	5	0.57
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	5	0.57
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	5	0.57
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	5	0.57
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	5	0.57
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	5	0.57
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	5	0.57
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	5	0.57
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	5	0.57
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	5	0.57
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	5	0.57
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	5	0.57
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	5	0.57
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	17	0.57
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	17	0.57
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	17	0.57
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	15	0.57
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	15	0.57
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	15	0.57
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	17	0.57
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	17	0.57
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	17	0.57
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	17	0.57
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	17	0.57
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	17	0.57
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	11	0.57
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	11	0.57
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	1	0.57
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	2	0.57
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	15	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	16	0.57
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	8	0.56
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	8	0.56
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	8	0.56
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	8	0.56
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	8	0.56
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	8	0.56
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	1	0.56
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	1	0.56
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	1	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	7	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	7	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	7	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	7	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	7	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	7	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	7	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	7	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	7	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	7	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	7	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	7	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	7	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	7	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	7	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	7	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	7	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	7	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	7	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	7	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	7	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	7	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	7	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	7	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	7	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	7	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	7	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	7	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	7	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	7	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	7	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	7	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	7	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	7	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	7	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	20	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	20	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	20	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	20	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	20	0.56
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	20	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	20	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	20	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	20	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	20	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	20	0.56
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	20	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	20	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	20	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	20	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	20	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	20	0.56
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	20	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	20	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	20	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	20	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	20	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	20	0.56
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	20	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	20	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	20	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	20	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	20	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	20	0.56
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	20	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	20	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	20	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	20	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	20	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	20	0.56
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	20	0.56
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	19	0.56
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	19	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	19	0.56
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	19	0.56
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	19	0.56
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	19	0.56
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	19	0.56
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	19	0.56
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	19	0.56
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	19	0.56
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	19	0.56
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	19	0.56
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	14	0.56
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	14	0.56
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	14	0.56
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	14	0.56
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	14	0.56
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	14	0.56
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	7	0.56
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	18	0.56
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	5	0.55
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	5	0.55
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	5	0.55
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	5	0.55
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	5	0.55
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	5	0.55
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	19	0.55
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	19	0.55
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	19	0.55
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	19	0.55
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	19	0.55
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	19	0.55
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	1	0.55
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	2	0.55
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	9	0.55
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	8	0.55
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	19	0.55
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	14	0.54
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	14	0.54
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	14	0.54
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	13	0.54
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	13	0.54
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	13	0.54
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	13	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	13	0.54
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	13	0.54
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	13	0.54
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	13	0.54
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	13	0.54
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	13	0.54
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	13	0.54
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	13	0.54
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	13	0.54
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	13	0.54
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	13	0.54
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	13	0.54
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	13	0.54
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	13	0.54
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	13	0.54
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	13	0.54
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	13	0.54
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	13	0.54
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	13	0.54
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	13	0.54
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	13	0.54
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	13	0.54
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	13	0.54
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	13	0.54
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	13	0.54
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	13	0.54
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	13	0.54
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	13	0.54
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	13	0.54
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	13	0.54
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	13	0.54
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	13	0.54
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	16	0.54
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	16	0.54
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	16	0.54
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	16	0.54
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	16	0.54
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	16	0.54
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	8	0.54
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	8	0.54
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	8	0.54
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	8	0.54
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	8	0.54
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	2	0.54
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	2	0.54
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	2	0.54
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	2	0.54
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	2	0.54
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	2	0.54
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	2	0.54
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	2	0.54
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	2	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	8	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	8	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	8	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	8	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	8	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	8	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	8	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	8	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	8	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	11	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	11	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	11	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	11	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	11	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	11	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	11	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	11	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	11	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	20	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	20	0.54
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	20	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	20	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	20	0.54
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	20	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	20	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	20	0.54
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	20	0.54
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	16	0.54
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	16	0.54
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	16	0.54
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	14	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	6	0.53
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	6	0.53
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	6	0.53
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	6	0.53
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	6	0.53
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	6	0.53
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	4	0.53
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	4	0.53
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	4	0.53
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	17	0.53
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	17	0.53
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	17	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	12	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	12	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	12	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	12	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	12	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	12	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	17	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	17	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	17	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	17	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	17	0.53
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	17	0.53
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	9	0.53
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	9	0.53
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	9	0.53
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	9	0.53
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	9	0.53
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	9	0.53
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	5	0.53
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	5	0.53
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	5	0.53
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	5	0.53
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	5	0.53
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	5	0.53
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	5	0.53
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	5	0.53
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	5	0.53
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	9	0.53
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	9	0.53
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	5	0.53
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	6	0.53
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	19	0.53
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	5	0.53
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	7	0.53
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	6	0.53
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	16	0.53
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	20	0.53
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	7	0.53
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	19	0.53
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	2	0.52
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	2	0.52
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	2	0.52
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	3	0.52
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	3	0.52
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	3	0.52
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	16	0.52
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	16	0.52
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	16	0.52
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	16	0.52
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	3	0.52
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	3	0.52
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	3	0.52
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	3	0.52
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	3	0.52
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	3	0.52
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	7	0.52
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	7	0.52
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	7	0.52
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	7	0.52
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	7	0.52
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	7	0.52
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	7	0.52
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	7	0.52
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	7	0.52
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	14	0.52
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	14	0.52
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	14	0.52
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	20	0.52
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	20	0.52
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	20	0.52
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	4	0.52
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	4	0.52
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	13	0.52
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	13	0.52
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	1	0.52
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	17	0.52
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	14	0.52
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	16	0.52
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	5	0.52
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	14	0.52
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	1	0.52
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	12	0.52
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	16	0.51
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	16	0.51
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	16	0.51
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	16	0.51
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	16	0.51
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	16	0.51
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	16	0.51
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	16	0.51
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	16	0.51
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	16	0.51
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	16	0.51
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	16	0.51
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	16	0.51
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	16	0.51
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	16	0.51
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	16	0.51
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	16	0.51
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	16	0.51
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	16	0.51
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	16	0.51
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	16	0.51
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	16	0.51
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	16	0.51
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	16	0.51
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	16	0.51
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	16	0.51
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	16	0.51
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	16	0.51
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	16	0.51
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	16	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	16	0.51
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	16	0.51
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	16	0.51
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	16	0.51
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	16	0.51
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	16	0.51
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	1	0.51
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	1	0.51
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	1	0.51
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	1	0.51
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	1	0.51
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	1	0.51
(1,434)	1:50:A:VAL:HG11	1:152:A:TRP:H	2	0.51
(1,434)	1:50:A:VAL:HG12	1:152:A:TRP:H	2	0.51
(1,434)	1:50:A:VAL:HG13	1:152:A:TRP:H	2	0.51
(1,434)	1:50:A:VAL:HG21	1:152:A:TRP:H	2	0.51
(1,434)	1:50:A:VAL:HG22	1:152:A:TRP:H	2	0.51
(1,434)	1:50:A:VAL:HG23	1:152:A:TRP:H	2	0.51
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	11	0.51
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	11	0.51
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	11	0.51
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	11	0.51
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	11	0.51
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	11	0.51
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	14	0.51
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	14	0.51
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	14	0.51
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	14	0.51
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	14	0.51
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	14	0.51
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	13	0.51
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	13	0.51
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	13	0.51
(1,378)	1:17:A:LEU:HD11	1:113:A:ALA:H	18	0.51
(1,378)	1:17:A:LEU:HD12	1:113:A:ALA:H	18	0.51
(1,378)	1:17:A:LEU:HD13	1:113:A:ALA:H	18	0.51
(1,378)	1:17:A:LEU:HD21	1:113:A:ALA:H	18	0.51
(1,378)	1:17:A:LEU:HD22	1:113:A:ALA:H	18	0.51
(1,378)	1:17:A:LEU:HD23	1:113:A:ALA:H	18	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	3	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	3	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	3	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	3	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	3	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	3	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	3	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	3	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	6	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	6	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	6	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	6	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	6	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	6	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	6	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	6	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	6	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	19	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	19	0.51
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	19	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	19	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	19	0.51
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	19	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	19	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	19	0.51
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	19	0.51
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	14	0.51
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	14	0.51
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	14	0.51
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	8	0.51
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	8	0.51
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	8	0.51
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	10	0.51
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	10	0.51
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	10	0.51
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	18	0.51
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	3	0.51
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	4	0.51
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	5	0.51
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	9	0.51
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	7	0.5
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	7	0.5
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	7	0.5
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:99:A:VAL:HG11	1:145:A:TRP:H	9	0.5
(1,475)	1:99:A:VAL:HG12	1:145:A:TRP:H	9	0.5
(1,475)	1:99:A:VAL:HG13	1:145:A:TRP:H	9	0.5
(1,475)	1:99:A:VAL:HG21	1:145:A:TRP:H	9	0.5
(1,475)	1:99:A:VAL:HG22	1:145:A:TRP:H	9	0.5
(1,475)	1:99:A:VAL:HG23	1:145:A:TRP:H	9	0.5
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	14	0.5
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	14	0.5
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	14	0.5
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	14	0.5
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	14	0.5
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	14	0.5
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	14	0.5
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	14	0.5
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	14	0.5
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	14	0.5
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	14	0.5
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	14	0.5
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	14	0.5
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	14	0.5
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	14	0.5
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	14	0.5
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	14	0.5
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	14	0.5
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	14	0.5
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	14	0.5
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	14	0.5
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	14	0.5
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	14	0.5
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	14	0.5
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	14	0.5
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	14	0.5
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	14	0.5
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	14	0.5
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	14	0.5
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	14	0.5
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	14	0.5
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	14	0.5
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	14	0.5
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	14	0.5
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	14	0.5
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	14	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	6	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	6	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	6	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	6	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	6	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	6	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	18	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	18	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	18	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	18	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	18	0.5
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	18	0.5
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	7	0.5
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	7	0.5
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	7	0.5
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	7	0.5
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	7	0.5
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	7	0.5
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	8	0.5
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	8	0.5
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	8	0.5
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	8	0.5
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	8	0.5
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	8	0.5
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	4	0.5
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	4	0.5
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	4	0.5
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	4	0.5
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	4	0.5
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	4	0.5
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	13	0.5
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	13	0.5
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	13	0.5
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	13	0.5
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	13	0.5
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	13	0.5
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	14	0.5
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	14	0.5
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	14	0.5
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	14	0.5
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	14	0.5
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	14	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	3	0.5
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	8	0.5
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	18	0.5
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	19	0.5
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	12	0.5
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	16	0.5
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	11	0.5
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	13	0.5
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	17	0.5
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	7	0.5
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	15	0.5
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	16	0.5
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	10	0.49
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	10	0.49
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	10	0.49
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	11	0.49
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	11	0.49
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	11	0.49
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	14	0.49
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	14	0.49
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	14	0.49
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	14	0.49
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	14	0.49
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	14	0.49
(1,421)	1:21:A:LEU:HD11	1:26:A:TYR:H	6	0.49
(1,421)	1:21:A:LEU:HD12	1:26:A:TYR:H	6	0.49
(1,421)	1:21:A:LEU:HD13	1:26:A:TYR:H	6	0.49
(1,421)	1:21:A:LEU:HD21	1:26:A:TYR:H	6	0.49
(1,421)	1:21:A:LEU:HD22	1:26:A:TYR:H	6	0.49
(1,421)	1:21:A:LEU:HD23	1:26:A:TYR:H	6	0.49
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	2	0.49
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	2	0.49
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	2	0.49
(1,371)	1:13:A:VAL:HG21	1:134:A:MET:H	13	0.49
(1,371)	1:13:A:VAL:HG22	1:134:A:MET:H	13	0.49
(1,371)	1:13:A:VAL:HG23	1:134:A:MET:H	13	0.49
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	12	0.49
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	12	0.49
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	12	0.49
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	12	0.49
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	12	0.49
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	12	0.49
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	12	0.49
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	12	0.49
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	3	0.49
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	3	0.49
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	3	0.49
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	3	0.49
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	3	0.49
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	3	0.49
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	4	0.49
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	4	0.49
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	4	0.49
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	4	0.49
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	4	0.49
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	4	0.49
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	8	0.49
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	11	0.49
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	17	0.49
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	19	0.49
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	2	0.49
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	5	0.49
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	7	0.49
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	17	0.49
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	20	0.49
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	5	0.49
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	14	0.49
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	2	0.49
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	6	0.48
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	6	0.48
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	6	0.48
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	3	0.48
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	8	0.48
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	18	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG11	12	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG12	12	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG13	12	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG21	12	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG22	12	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG23	12	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG11	12	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG12	12	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG13	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG21	12	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG22	12	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG23	12	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG11	12	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG12	12	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG13	12	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG21	12	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG22	12	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG23	12	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG11	12	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG12	12	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG13	12	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG21	12	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG22	12	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG23	12	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG11	12	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG12	12	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG13	12	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG21	12	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG22	12	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG23	12	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG11	12	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG12	12	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG13	12	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG21	12	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG22	12	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG23	12	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG11	17	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG12	17	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG13	17	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG21	17	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG22	17	0.48
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG23	17	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG11	17	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG12	17	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG13	17	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG21	17	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG22	17	0.48
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG23	17	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG11	17	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG12	17	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG13	17	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG21	17	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG22	17	0.48
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG23	17	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG11	17	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG12	17	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG13	17	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG21	17	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG22	17	0.48
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG23	17	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG11	17	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG12	17	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG13	17	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG21	17	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG22	17	0.48
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG23	17	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG11	17	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG12	17	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG13	17	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG21	17	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG22	17	0.48
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG23	17	0.48
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	5	0.48
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	5	0.48
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	5	0.48
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	5	0.48
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	5	0.48
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	5	0.48
(1,454)	1:72:A:LEU:HD11	1:111:A:GLY:H	9	0.48
(1,454)	1:72:A:LEU:HD12	1:111:A:GLY:H	9	0.48
(1,454)	1:72:A:LEU:HD13	1:111:A:GLY:H	9	0.48
(1,454)	1:72:A:LEU:HD21	1:111:A:GLY:H	9	0.48
(1,454)	1:72:A:LEU:HD22	1:111:A:GLY:H	9	0.48
(1,454)	1:72:A:LEU:HD23	1:111:A:GLY:H	9	0.48
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	20	0.48
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	20	0.48
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	20	0.48
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	20	0.48
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	20	0.48
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	20	0.48
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	4	0.48
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	4	0.48
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	4	0.48
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	4	0.48
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	4	0.48
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	1	0.48
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	15	0.48
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	2	0.48
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	9	0.48
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	18	0.48
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	7	0.48
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	16	0.48
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	15	0.47
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	15	0.47
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	15	0.47
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	9	0.47
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	9	0.47
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	9	0.47
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	9	0.47
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	9	0.47
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	9	0.47
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	9	0.47
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	9	0.47
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	9	0.47
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	9	0.47
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	9	0.47
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	9	0.47
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	9	0.47
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	9	0.47
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	9	0.47
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	9	0.47
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	9	0.47
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	9	0.47
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	9	0.47
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	9	0.47
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	9	0.47
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	9	0.47
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	9	0.47
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	9	0.47
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	9	0.47
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	9	0.47
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	9	0.47
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	9	0.47
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	9	0.47
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	9	0.47
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	9	0.47
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	9	0.47
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	9	0.47
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	9	0.47
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	9	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	9	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	9	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	9	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	9	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	9	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	9	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	15	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	15	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	15	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	15	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	15	0.47
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	15	0.47
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	14	0.47
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	14	0.47
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	14	0.47
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	14	0.47
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	14	0.47
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	14	0.47
(1,377)	1:17:A:LEU:HD11	1:111:A:GLY:H	3	0.47
(1,377)	1:17:A:LEU:HD12	1:111:A:GLY:H	3	0.47
(1,377)	1:17:A:LEU:HD13	1:111:A:GLY:H	3	0.47
(1,377)	1:17:A:LEU:HD21	1:111:A:GLY:H	3	0.47
(1,377)	1:17:A:LEU:HD22	1:111:A:GLY:H	3	0.47
(1,377)	1:17:A:LEU:HD23	1:111:A:GLY:H	3	0.47
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	14	0.47
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	14	0.47
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	14	0.47
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	16	0.47
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	16	0.47
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	16	0.47
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD21	8	0.47
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD22	8	0.47
(1,290)	1:16:A:PHE:H	1:54:A:LEU:HD23	8	0.47
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	11	0.47
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	19	0.47
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	17	0.47
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	13	0.47
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	18	0.47
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	15	0.47
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	2	0.46
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	2	0.46
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	2	0.46
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	2	0.46
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	2	0.46
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	2	0.46
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	5	0.46
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	5	0.46
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	5	0.46
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	17	0.46
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	17	0.46
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	17	0.46
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	17	0.46
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	17	0.46
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	17	0.46
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	17	0.46
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	17	0.46
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	17	0.46
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	17	0.46
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	17	0.46
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	17	0.46
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	17	0.46
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	17	0.46
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	17	0.46
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	17	0.46
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	17	0.46
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	17	0.46
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	17	0.46
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	17	0.46
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	17	0.46
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	17	0.46
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	17	0.46
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	17	0.46
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	17	0.46
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	17	0.46
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	17	0.46
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	17	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	17	0.46
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	17	0.46
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	17	0.46
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	17	0.46
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	17	0.46
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	17	0.46
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	17	0.46
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	17	0.46
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	8	0.46
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	8	0.46
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	8	0.46
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	8	0.46
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	8	0.46
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	8	0.46
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	2	0.46
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	2	0.46
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	2	0.46
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	2	0.46
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	2	0.46
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	2	0.46
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD11	17	0.46
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD12	17	0.46
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD13	17	0.46
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD21	17	0.46
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD22	17	0.46
(1,419)	1:18:A:SER:H	1:54:A:LEU:HD23	17	0.46
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	9	0.46
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	9	0.46
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	9	0.46
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD11	11	0.46
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD12	11	0.46
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD13	11	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG11	12	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG12	12	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG13	12	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG21	12	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG22	12	0.46
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG23	12	0.46
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	9	0.46
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	9	0.46
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	9	0.46
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	18	0.46
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	9	0.46
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	11	0.46
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	18	0.46
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	14	0.46
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	2	0.46
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	10	0.46
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	13	0.46
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	2	0.46
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	15	0.45
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	15	0.45
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	15	0.45
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	15	0.45
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	15	0.45
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	15	0.45
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	17	0.45
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	12	0.45
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	12	0.45
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	12	0.45
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	12	0.45
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	12	0.45
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	12	0.45
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	12	0.45
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	12	0.45
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	12	0.45
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	12	0.45
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	12	0.45
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	12	0.45
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	12	0.45
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	12	0.45
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	12	0.45
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	12	0.45
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	12	0.45
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	12	0.45
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	12	0.45
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	12	0.45
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	12	0.45
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	12	0.45
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	12	0.45
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	12	0.45
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	12	0.45
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	12	0.45
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	12	0.45
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	12	0.45
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	12	0.45
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	12	0.45
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	12	0.45
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	12	0.45
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	12	0.45
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	12	0.45
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	12	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	3	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	3	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	3	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	3	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	3	0.45
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	3	0.45
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD11	14	0.45
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD12	14	0.45
(1,396)	1:138:A:LEU:HD11	1:146:A:ILE:HD13	14	0.45
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD11	14	0.45
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD12	14	0.45
(1,396)	1:138:A:LEU:HD12	1:146:A:ILE:HD13	14	0.45
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD11	14	0.45
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD12	14	0.45
(1,396)	1:138:A:LEU:HD13	1:146:A:ILE:HD13	14	0.45
(1,362)	1:72:A:LEU:HD21	1:110:A:PHE:H	1	0.45
(1,362)	1:72:A:LEU:HD22	1:110:A:PHE:H	1	0.45
(1,362)	1:72:A:LEU:HD23	1:110:A:PHE:H	1	0.45
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG11	20	0.45
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG12	20	0.45
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG13	20	0.45
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG21	20	0.45
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG22	20	0.45
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG23	20	0.45
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	10	0.45
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	10	0.45
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	10	0.45
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	13	0.45
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	13	0.45
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	13	0.45
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	16	0.45
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	14	0.45
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	3	0.45
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	15	0.45
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	19	0.45
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	1	0.45
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	6	0.45
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	10	0.45
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	20	0.45
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	13	0.45
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	1	0.45
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	8	0.44
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	8	0.44
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	8	0.44
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	8	0.44
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	8	0.44
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	8	0.44
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	8	0.44
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	8	0.44
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	8	0.44
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	8	0.44
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	8	0.44
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	8	0.44
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	8	0.44
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	8	0.44
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	8	0.44
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	8	0.44
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	8	0.44
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	8	0.44
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	8	0.44
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	8	0.44
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	8	0.44
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	8	0.44
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	8	0.44
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	8	0.44
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	8	0.44
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	8	0.44
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	8	0.44
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	8	0.44
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	8	0.44
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	8	0.44
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	8	0.44
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	8	0.44
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	8	0.44
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	8	0.44
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	8	0.44
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD11	10	0.44
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD12	10	0.44
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD13	10	0.44
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD21	10	0.44
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD22	10	0.44
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD23	10	0.44
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	7	0.44
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	7	0.44
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	7	0.44
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	10	0.44
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	16	0.44
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	12	0.44
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	13	0.44
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	20	0.44
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	1	0.44
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	2	0.44
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	7	0.44
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	12	0.43
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	12	0.43
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	12	0.43
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	13	0.43
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	13	0.43
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	13	0.43
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	13	0.43
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	13	0.43
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	13	0.43
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	11	0.43
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	11	0.43
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	11	0.43
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	7	0.43
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	6	0.43
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	14	0.43
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	15	0.43
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	6	0.43
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	11	0.43
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	3	0.43
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	1	0.43
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	19	0.43
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	3	0.43
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	12	0.43
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	19	0.43
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	3	0.43
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	12	0.43
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	8	0.43
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	15	0.43
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	6	0.43
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	9	0.43
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	5	0.43
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	17	0.43
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	16	0.42
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	16	0.42
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	16	0.42
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	18	0.42
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	18	0.42
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	18	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	15	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	15	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	15	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	15	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	15	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	15	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	15	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	15	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	15	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	15	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	15	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	15	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	15	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	15	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	15	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	15	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	15	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	15	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	15	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	15	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	15	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	15	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	15	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	15	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	15	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	15	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	15	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	15	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	15	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	15	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	15	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	15	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	15	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	15	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	15	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	18	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	18	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	18	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	18	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	18	0.42
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	18	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	18	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	18	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	18	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	18	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	18	0.42
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	18	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	18	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	18	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	18	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	18	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	18	0.42
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	18	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	18	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	18	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	18	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	18	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	18	0.42
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	18	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	18	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	18	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	18	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	18	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	18	0.42
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	18	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	18	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	18	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	18	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	18	0.42
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	18	0.42
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	4	0.42
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	4	0.42
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	4	0.42
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	4	0.42
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	4	0.42
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	4	0.42
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	12	0.42
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	12	0.42
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	12	0.42
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	12	0.42
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	12	0.42
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	12	0.42
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	4	0.42
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	4	0.42
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	4	0.42
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	7	0.42
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	7	0.42
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	7	0.42
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	14	0.42
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	14	0.42
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	14	0.42
(1,238)	1:134:A:MET:H	1:136:A:THR:H	10	0.42
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	18	0.42
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	2	0.42
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	3	0.42
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	4	0.42
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	12	0.42
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	5	0.42
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	7	0.42
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	9	0.42
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	16	0.42
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	7	0.42
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	9	0.42
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	17	0.42
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	8	0.42
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	11	0.42
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	5	0.42
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	8	0.42
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	3	0.42
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	4	0.42
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	10	0.42
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	11	0.42
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	15	0.41
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	15	0.41
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	15	0.41
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	15	0.41
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	15	0.41
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	15	0.41
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	15	0.41
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	15	0.41
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	15	0.41
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	15	0.41
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	15	0.41
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	15	0.41
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	15	0.41
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	15	0.41
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	15	0.41
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	15	0.41
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	15	0.41
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	15	0.41
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	15	0.41
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	15	0.41
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	15	0.41
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	15	0.41
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	15	0.41
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	15	0.41
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	15	0.41
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	15	0.41
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	15	0.41
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	15	0.41
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	15	0.41
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	15	0.41
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	15	0.41
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	15	0.41
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	15	0.41
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	15	0.41
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	15	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	15	0.41
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	17	0.41
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	17	0.41
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	17	0.41
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	17	0.41
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	17	0.41
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	17	0.41
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	17	0.41
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	17	0.41
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	17	0.41
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	17	0.41
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	17	0.41
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	17	0.41
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	17	0.41
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	17	0.41
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	17	0.41
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	17	0.41
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	17	0.41
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	17	0.41
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	17	0.41
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	17	0.41
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	17	0.41
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	17	0.41
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	17	0.41
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	17	0.41
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	17	0.41
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	17	0.41
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	17	0.41
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	17	0.41
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	17	0.41
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	17	0.41
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	17	0.41
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	17	0.41
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	17	0.41
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	17	0.41
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	17	0.41
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	17	0.41
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	11	0.41
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	11	0.41
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	11	0.41
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	11	0.41
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	11	0.41
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	9	0.41
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	9	0.41
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	9	0.41
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	9	0.41
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	9	0.41
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	9	0.41
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	18	0.41
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	18	0.41
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	18	0.41
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	5	0.41
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	5	0.41
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	5	0.41
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	5	0.41
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	5	0.41
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	5	0.41
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	5	0.41
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	5	0.41
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	5	0.41
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	18	0.41
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	18	0.41
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	18	0.41
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	18	0.41
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	18	0.41
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	18	0.41
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	9	0.41
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	9	0.41
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	9	0.41
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	11	0.41
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	11	0.41
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	11	0.41
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	12	0.41
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	20	0.41
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	5	0.41
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	6	0.41
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	16	0.41
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	8	0.41
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	15	0.41
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	6	0.41
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	17	0.41
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	20	0.41
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	19	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	5	0.41
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	19	0.41
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	18	0.41
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	20	0.41
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	12	0.41
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	20	0.41
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	13	0.41
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	18	0.41
(1,79)	1:27:A:SER:H	1:30:A:GLN:H	8	0.41
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	5	0.41
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	5	0.41
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	9	0.41
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	4	0.41
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	13	0.41
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	14	0.41
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	3	0.4
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	3	0.4
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	3	0.4
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	3	0.4
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	3	0.4
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	3	0.4
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	2	0.4
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	2	0.4
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	2	0.4
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	2	0.4
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	2	0.4
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	2	0.4
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	2	0.4
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	2	0.4
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	2	0.4
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	2	0.4
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	2	0.4
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	2	0.4
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	2	0.4
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	2	0.4
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	2	0.4
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	2	0.4
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	2	0.4
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	2	0.4
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	2	0.4
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	2	0.4
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	2	0.4
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	2	0.4
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	2	0.4
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	2	0.4
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	2	0.4
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	2	0.4
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	2	0.4
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	2	0.4
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	2	0.4
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	2	0.4
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	2	0.4
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	2	0.4
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	2	0.4
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	2	0.4
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	2	0.4
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	17	0.4
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	17	0.4
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	17	0.4
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	17	0.4
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	17	0.4
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	17	0.4
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	18	0.4
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	18	0.4
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	18	0.4
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	18	0.4
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	18	0.4
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	18	0.4
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	7	0.4
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	7	0.4
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	7	0.4
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	12	0.4
(1,238)	1:134:A:MET:H	1:136:A:THR:H	12	0.4
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	1	0.4
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	4	0.4
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	9	0.4
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	10	0.4
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	5	0.4
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	13	0.4
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	1	0.4
(1,213)	1:23:A:GLN:H	1:25:A:GLY:H	19	0.4
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	9	0.4
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	17	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	20	0.4
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	3	0.4
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	5	0.4
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	2	0.4
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	7	0.4
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	16	0.4
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	10	0.4
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	12	0.4
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	2	0.4
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	6	0.4
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	14	0.4
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	18	0.4
(2,8)	1:78:A:ILE:HD11	1:129:A:ARG:H	9	0.39
(2,8)	1:78:A:ILE:HD12	1:129:A:ARG:H	9	0.39
(2,8)	1:78:A:ILE:HD13	1:129:A:ARG:H	9	0.39
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	12	0.39
(1,498)	1:126:A:LEU:HD11	1:130:A:ILE:HD11	12	0.39
(1,498)	1:126:A:LEU:HD11	1:130:A:ILE:HD12	12	0.39
(1,498)	1:126:A:LEU:HD11	1:130:A:ILE:HD13	12	0.39
(1,498)	1:126:A:LEU:HD12	1:130:A:ILE:HD11	12	0.39
(1,498)	1:126:A:LEU:HD12	1:130:A:ILE:HD12	12	0.39
(1,498)	1:126:A:LEU:HD12	1:130:A:ILE:HD13	12	0.39
(1,498)	1:126:A:LEU:HD13	1:130:A:ILE:HD11	12	0.39
(1,498)	1:126:A:LEU:HD13	1:130:A:ILE:HD12	12	0.39
(1,498)	1:126:A:LEU:HD13	1:130:A:ILE:HD13	12	0.39
(1,498)	1:126:A:LEU:HD21	1:130:A:ILE:HD11	12	0.39
(1,498)	1:126:A:LEU:HD21	1:130:A:ILE:HD12	12	0.39
(1,498)	1:126:A:LEU:HD21	1:130:A:ILE:HD13	12	0.39
(1,498)	1:126:A:LEU:HD22	1:130:A:ILE:HD11	12	0.39
(1,498)	1:126:A:LEU:HD22	1:130:A:ILE:HD12	12	0.39
(1,498)	1:126:A:LEU:HD22	1:130:A:ILE:HD13	12	0.39
(1,498)	1:126:A:LEU:HD23	1:130:A:ILE:HD11	12	0.39
(1,498)	1:126:A:LEU:HD23	1:130:A:ILE:HD12	12	0.39
(1,498)	1:126:A:LEU:HD23	1:130:A:ILE:HD13	12	0.39
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	9	0.39
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	9	0.39
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	9	0.39
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	9	0.39
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	9	0.39
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	9	0.39
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	9	0.39
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	9	0.39
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	9	0.39
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	9	0.39
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	9	0.39
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	9	0.39
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	9	0.39
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	9	0.39
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	9	0.39
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	9	0.39
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	9	0.39
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	9	0.39
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	9	0.39
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	9	0.39
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	9	0.39
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	9	0.39
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	9	0.39
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	9	0.39
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	9	0.39
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	9	0.39
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	9	0.39
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	9	0.39
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	9	0.39
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	9	0.39
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	9	0.39
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	9	0.39
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	9	0.39
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	9	0.39
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	9	0.39
(1,466)	1:94:A:LEU:HD11	1:106:A:ALA:H	10	0.39
(1,466)	1:94:A:LEU:HD12	1:106:A:ALA:H	10	0.39
(1,466)	1:94:A:LEU:HD13	1:106:A:ALA:H	10	0.39
(1,466)	1:94:A:LEU:HD21	1:106:A:ALA:H	10	0.39
(1,466)	1:94:A:LEU:HD22	1:106:A:ALA:H	10	0.39
(1,466)	1:94:A:LEU:HD23	1:106:A:ALA:H	10	0.39
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	5	0.39
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	5	0.39
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	5	0.39
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	5	0.39
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	5	0.39
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	5	0.39
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	5	0.39
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	5	0.39
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	5	0.39
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	5	0.39
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	5	0.39
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	5	0.39
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	5	0.39
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	5	0.39
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	5	0.39
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	5	0.39
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	5	0.39
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	5	0.39
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	5	0.39
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	5	0.39
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	5	0.39
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	5	0.39
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	5	0.39
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	5	0.39
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	5	0.39
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	5	0.39
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	5	0.39
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	5	0.39
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	5	0.39
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	5	0.39
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	5	0.39
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	5	0.39
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	5	0.39
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	5	0.39
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	5	0.39
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	20	0.39
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	20	0.39
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	20	0.39
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	20	0.39
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	20	0.39
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	20	0.39
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	6	0.39
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	6	0.39
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	6	0.39
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	6	0.39
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	6	0.39
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	6	0.39
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	19	0.39
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	19	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	19	0.39
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	19	0.39
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	19	0.39
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	19	0.39
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	2	0.39
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	2	0.39
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	2	0.39
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	13	0.39
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	13	0.39
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	13	0.39
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	20	0.39
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	20	0.39
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	20	0.39
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	20	0.39
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	20	0.39
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	20	0.39
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	4	0.39
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	16	0.39
(1,238)	1:134:A:MET:H	1:136:A:THR:H	13	0.39
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	3	0.39
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	13	0.39
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	11	0.39
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	12	0.39
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	10	0.39
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	14	0.39
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	17	0.39
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	4	0.39
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	15	0.39
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	12	0.39
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	11	0.39
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	16	0.39
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	18	0.39
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	1	0.39
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	1	0.39
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	9	0.39
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	16	0.39
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	4	0.39
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	2	0.39
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	8	0.39
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	16	0.39
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD11	13	0.38
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD12	13	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD13	13	0.38
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD21	13	0.38
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD22	13	0.38
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD23	13	0.38
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	6	0.38
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	6	0.38
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	6	0.38
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	6	0.38
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	6	0.38
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	6	0.38
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	6	0.38
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	6	0.38
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	6	0.38
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	6	0.38
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	6	0.38
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	6	0.38
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	6	0.38
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	6	0.38
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	6	0.38
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	6	0.38
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	6	0.38
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	6	0.38
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	6	0.38
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	6	0.38
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	6	0.38
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	6	0.38
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	6	0.38
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	6	0.38
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	6	0.38
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	6	0.38
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	6	0.38
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	6	0.38
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	6	0.38
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	6	0.38
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	6	0.38
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	6	0.38
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	6	0.38
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	6	0.38
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	6	0.38
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	6	0.38
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	14	0.38
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	14	0.38
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	14	0.38
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	14	0.38
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	14	0.38
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	5	0.38
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	5	0.38
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	5	0.38
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	5	0.38
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	5	0.38
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	5	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	4	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	4	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	4	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	4	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	4	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	4	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	4	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	4	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	4	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	4	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	4	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	4	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	4	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	4	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	4	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	4	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	4	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	4	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	4	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	4	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	4	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	4	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	4	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	4	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	4	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	4	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	4	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	4	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	4	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	4	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	4	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	4	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	4	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	4	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	4	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	7	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	7	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	7	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	7	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	7	0.38
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	7	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	7	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	7	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	7	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	7	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	7	0.38
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	7	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	7	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	7	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	7	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	7	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	7	0.38
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	7	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	7	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	7	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	7	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	7	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	7	0.38
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	7	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	7	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	7	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	7	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	7	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	7	0.38
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	7	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	7	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	7	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	7	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	7	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	7	0.38
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	7	0.38
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	7	0.38
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	7	0.38
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	7	0.38
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	7	0.38
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	7	0.38
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	12	0.38
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	12	0.38
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	12	0.38
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	12	0.38
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	12	0.38
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	12	0.38
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG11	19	0.38
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG12	19	0.38
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG13	19	0.38
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG21	19	0.38
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG22	19	0.38
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG23	19	0.38
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG11	19	0.38
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG12	19	0.38
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG13	19	0.38
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG21	19	0.38
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG22	19	0.38
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG23	19	0.38
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG11	19	0.38
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG12	19	0.38
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG13	19	0.38
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG21	19	0.38
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG22	19	0.38
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG23	19	0.38
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG11	19	0.38
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG12	19	0.38
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG13	19	0.38
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG21	19	0.38
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG22	19	0.38
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG23	19	0.38
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG11	19	0.38
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG12	19	0.38
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG13	19	0.38
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG21	19	0.38
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG22	19	0.38
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG23	19	0.38
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG11	19	0.38
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG12	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG13	19	0.38
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG21	19	0.38
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG22	19	0.38
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG23	19	0.38
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	14	0.38
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	14	0.38
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	14	0.38
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	7	0.38
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	7	0.38
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	7	0.38
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	7	0.38
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	7	0.38
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	7	0.38
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	7	0.38
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	7	0.38
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	7	0.38
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	12	0.38
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	12	0.38
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	12	0.38
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	12	0.38
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	12	0.38
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	12	0.38
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	5	0.38
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	5	0.38
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	13	0.38
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	15	0.38
(1,238)	1:134:A:MET:H	1:136:A:THR:H	4	0.38
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	2	0.38
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	7	0.38
(1,221)	1:125:A:VAL:H	1:127:A:VAL:H	12	0.38
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	13	0.38
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	18	0.38
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	8	0.38
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	19	0.38
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	8	0.38
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	15	0.38
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	15	0.38
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	4	0.38
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	6	0.38
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	14	0.38
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	20	0.38
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	16	0.37
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	16	0.37
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	16	0.37
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	16	0.37
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	16	0.37
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	16	0.37
(1,448)	1:72:A:LEU:HD11	1:90:A:VAL:H	6	0.37
(1,448)	1:72:A:LEU:HD12	1:90:A:VAL:H	6	0.37
(1,448)	1:72:A:LEU:HD13	1:90:A:VAL:H	6	0.37
(1,448)	1:72:A:LEU:HD21	1:90:A:VAL:H	6	0.37
(1,448)	1:72:A:LEU:HD22	1:90:A:VAL:H	6	0.37
(1,448)	1:72:A:LEU:HD23	1:90:A:VAL:H	6	0.37
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	6	0.37
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	6	0.37
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	6	0.37
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	6	0.37
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	6	0.37
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	6	0.37
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	19	0.37
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	19	0.37
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	19	0.37
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	19	0.37
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	19	0.37
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	19	0.37
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	19	0.37
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	19	0.37
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	19	0.37
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	19	0.37
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	19	0.37
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	19	0.37
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	19	0.37
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	19	0.37
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	19	0.37
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	19	0.37
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	19	0.37
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	19	0.37
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	19	0.37
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	19	0.37
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	19	0.37
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	19	0.37
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	19	0.37
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	19	0.37
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	19	0.37
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	19	0.37
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	19	0.37
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	19	0.37
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	19	0.37
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	19	0.37
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	19	0.37
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	19	0.37
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	19	0.37
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	19	0.37
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	19	0.37
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	7	0.37
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	7	0.37
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	7	0.37
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	7	0.37
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	7	0.37
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	7	0.37
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	8	0.37
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	8	0.37
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	8	0.37
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	8	0.37
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	8	0.37
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	8	0.37
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	14	0.37
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	14	0.37
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	14	0.37
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	14	0.37
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	14	0.37
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	14	0.37
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	15	0.37
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	15	0.37
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	15	0.37
(1,346)	1:143:A:GLU:H	1:146:A:ILE:HD11	12	0.37
(1,346)	1:143:A:GLU:H	1:146:A:ILE:HD12	12	0.37
(1,346)	1:143:A:GLU:H	1:146:A:ILE:HD13	12	0.37
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	5	0.37
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	5	0.37
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	5	0.37
(1,282)	1:12:A:LEU:HD11	1:51:A:LYS:H	6	0.37
(1,282)	1:12:A:LEU:HD12	1:51:A:LYS:H	6	0.37
(1,282)	1:12:A:LEU:HD13	1:51:A:LYS:H	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	20	0.37
(1,238)	1:134:A:MET:H	1:136:A:THR:H	19	0.37
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	6	0.37
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	3	0.37
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	10	0.37
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	15	0.37
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	11	0.37
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	18	0.37
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	1	0.37
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	6	0.37
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	6	0.37
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	11	0.37
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	7	0.37
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	20	0.37
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	9	0.37
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	1	0.37
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	2	0.37
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	11	0.37
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	15	0.37
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	18	0.37
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	14	0.37
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	17	0.37
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	12	0.37
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	19	0.37
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	20	0.37
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	4	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	4	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	4	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	4	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	4	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	4	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	12	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	12	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	12	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	12	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	12	0.36
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	12	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	1	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	1	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	1	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	1	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	1	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	1	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	1	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	1	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	1	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	1	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	1	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	1	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	1	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	1	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	1	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	1	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	1	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	1	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	1	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	1	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	1	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	1	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	1	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	1	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	1	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	1	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	1	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	1	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	1	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	1	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	1	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	1	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	1	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	1	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	1	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	2	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	2	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	2	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	2	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	2	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	2	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	2	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	2	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	2	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	2	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	2	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	2	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	2	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	2	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	2	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	2	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	2	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	2	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	2	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	2	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	2	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	2	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	2	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	2	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	2	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	2	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	2	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	2	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	2	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	2	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	2	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	2	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	2	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	2	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	2	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	6	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	6	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	6	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	6	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	6	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	6	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	6	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	6	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	6	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	6	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	6	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	6	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	6	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	6	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	6	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	6	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	6	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	6	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	6	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	6	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	6	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	6	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	6	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	6	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	6	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	6	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	6	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	6	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	6	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	6	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	6	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	6	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	6	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	6	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	6	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	10	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	10	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	10	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	10	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	10	0.36
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	10	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	10	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	10	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	10	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	10	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	10	0.36
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	10	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	10	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	10	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	10	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	10	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	10	0.36
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	10	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	10	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	10	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	10	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	10	0.36
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	10	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	10	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	10	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	10	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	10	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	10	0.36
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	10	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	10	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	10	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	10	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	10	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	10	0.36
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	10	0.36
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	20	0.36
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	20	0.36
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	20	0.36
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	20	0.36
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	20	0.36
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	20	0.36
(1,404)	1:12:A:LEU:HD11	1:152:A:TRP:HE1	11	0.36
(1,404)	1:12:A:LEU:HD12	1:152:A:TRP:HE1	11	0.36
(1,404)	1:12:A:LEU:HD13	1:152:A:TRP:HE1	11	0.36
(1,404)	1:12:A:LEU:HD21	1:152:A:TRP:HE1	11	0.36
(1,404)	1:12:A:LEU:HD22	1:152:A:TRP:HE1	11	0.36
(1,404)	1:12:A:LEU:HD23	1:152:A:TRP:HE1	11	0.36
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	7	0.36
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	16	0.36
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	16	0.36
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	17	0.36
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	12	0.36
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	14	0.36
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	16	0.36
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	8	0.36
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	11	0.36
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	9	0.36
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	19	0.36
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	15	0.36
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	17	0.36
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	3	0.36
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	7	0.36
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	4	0.36
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	15	0.36
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	10	0.36
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	14	0.36
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	8	0.36
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	7	0.36
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	8	0.36
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	16	0.36
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG11	9	0.35
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG12	9	0.35
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG13	9	0.35
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG21	9	0.35
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG22	9	0.35
(1,496)	1:126:A:LEU:HD11	1:127:A:VAL:HG23	9	0.35
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG11	9	0.35
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG12	9	0.35
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG13	9	0.35
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG21	9	0.35
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG22	9	0.35
(1,496)	1:126:A:LEU:HD12	1:127:A:VAL:HG23	9	0.35
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG11	9	0.35
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG12	9	0.35
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG13	9	0.35
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG21	9	0.35
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG22	9	0.35
(1,496)	1:126:A:LEU:HD13	1:127:A:VAL:HG23	9	0.35
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG11	9	0.35
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG12	9	0.35
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG13	9	0.35
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG21	9	0.35
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG22	9	0.35
(1,496)	1:126:A:LEU:HD21	1:127:A:VAL:HG23	9	0.35
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG11	9	0.35
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG12	9	0.35
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG13	9	0.35
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG21	9	0.35
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG22	9	0.35
(1,496)	1:126:A:LEU:HD22	1:127:A:VAL:HG23	9	0.35
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG11	9	0.35
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG12	9	0.35
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG13	9	0.35
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG21	9	0.35
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG22	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:126:A:LEU:HD23	1:127:A:VAL:HG23	9	0.35
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	11	0.35
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	11	0.35
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	11	0.35
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	11	0.35
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	11	0.35
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	11	0.35
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	11	0.35
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	11	0.35
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	11	0.35
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	11	0.35
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	11	0.35
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	11	0.35
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	11	0.35
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	11	0.35
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	11	0.35
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	11	0.35
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	11	0.35
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	11	0.35
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	11	0.35
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	11	0.35
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	11	0.35
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	11	0.35
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	11	0.35
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	11	0.35
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	11	0.35
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	11	0.35
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	11	0.35
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	11	0.35
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	11	0.35
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	11	0.35
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	11	0.35
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	11	0.35
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	11	0.35
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	11	0.35
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	11	0.35
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	11	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	13	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	13	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	13	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	13	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	13	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	13	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	13	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	13	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	13	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	13	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	13	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	13	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	13	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	13	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	13	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	13	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	13	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	13	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	13	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	13	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	13	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	13	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	13	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	13	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	13	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	13	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	13	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	13	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	13	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	13	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	13	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	13	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	13	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	13	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	13	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	20	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	20	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	20	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	20	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	20	0.35
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	20	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	20	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	20	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	20	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	20	0.35
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	20	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	20	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	20	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	20	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	20	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	20	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	20	0.35
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	20	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	20	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	20	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	20	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	20	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	20	0.35
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	20	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	20	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	20	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	20	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	20	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	20	0.35
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	20	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	20	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	20	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	20	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	20	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	20	0.35
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	20	0.35
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	4	0.35
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	4	0.35
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	4	0.35
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	4	0.35
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	4	0.35
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	4	0.35
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	4	0.35
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	4	0.35
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	4	0.35
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	4	0.35
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	4	0.35
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	4	0.35
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	13	0.35
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	13	0.35
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	13	0.35
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	13	0.35
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	13	0.35
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	20	0.35
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	20	0.35
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	20	0.35
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	20	0.35
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	20	0.35
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	20	0.35
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	3	0.35
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	5	0.35
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	9	0.35
(1,238)	1:134:A:MET:H	1:136:A:THR:H	6	0.35
(1,238)	1:134:A:MET:H	1:136:A:THR:H	14	0.35
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	8	0.35
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	19	0.35
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	18	0.35
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	20	0.35
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	18	0.35
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	11	0.35
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	17	0.35
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	20	0.35
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	10	0.35
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	3	0.35
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	1	0.35
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	10	0.35
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	12	0.35
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	1	0.35
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	13	0.35
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	14	0.35
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	4	0.35
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	19	0.35
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	3	0.35
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	2	0.35
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	8	0.35
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	20	0.35
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	16	0.35
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	1	0.35
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	13	0.35
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	5	0.35
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	17	0.35
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	3	0.35
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	18	0.35
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	7	0.34
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	7	0.34
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	7	0.34
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	7	0.34
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	7	0.34
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	1	0.34
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	8	0.34
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	8	0.34
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	8	0.34
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	8	0.34
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	8	0.34
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	8	0.34
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	4	0.34
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	4	0.34
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	4	0.34
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	4	0.34
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	4	0.34
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	4	0.34
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	11	0.34
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	11	0.34
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	11	0.34
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	11	0.34
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	11	0.34
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	11	0.34
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	11	0.34
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	11	0.34
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	11	0.34
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	11	0.34
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	11	0.34
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	11	0.34
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	11	0.34
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	11	0.34
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	11	0.34
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	11	0.34
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	11	0.34
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	11	0.34
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	11	0.34
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	11	0.34
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	11	0.34
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	11	0.34
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	11	0.34
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	11	0.34
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	11	0.34
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	11	0.34
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	11	0.34
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	11	0.34
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	11	0.34
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	11	0.34
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	11	0.34
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	11	0.34
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	11	0.34
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	11	0.34
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	11	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	1	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	1	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	1	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	1	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	1	0.34
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	1	0.34
(1,422)	1:21:A:LEU:HD11	1:28:A:TRP:H	20	0.34
(1,422)	1:21:A:LEU:HD12	1:28:A:TRP:H	20	0.34
(1,422)	1:21:A:LEU:HD13	1:28:A:TRP:H	20	0.34
(1,422)	1:21:A:LEU:HD21	1:28:A:TRP:H	20	0.34
(1,422)	1:21:A:LEU:HD22	1:28:A:TRP:H	20	0.34
(1,422)	1:21:A:LEU:HD23	1:28:A:TRP:H	20	0.34
(1,378)	1:17:A:LEU:HD11	1:113:A:ALA:H	19	0.34
(1,378)	1:17:A:LEU:HD12	1:113:A:ALA:H	19	0.34
(1,378)	1:17:A:LEU:HD13	1:113:A:ALA:H	19	0.34
(1,378)	1:17:A:LEU:HD21	1:113:A:ALA:H	19	0.34
(1,378)	1:17:A:LEU:HD22	1:113:A:ALA:H	19	0.34
(1,378)	1:17:A:LEU:HD23	1:113:A:ALA:H	19	0.34
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	11	0.34
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	18	0.34
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	5	0.34
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	8	0.34
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	20	0.34
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	11	0.34
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	3	0.34
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	10	0.34
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	18	0.34
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	13	0.34
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	1	0.34
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	17	0.34
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	2	0.34
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	6	0.34
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	8	0.34
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	13	0.34
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	15	0.34
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	1	0.34
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	3	0.34
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	20	0.34
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	3	0.34
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	11	0.34
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	18	0.34
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	2	0.34
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	7	0.34
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	8	0.34
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	13	0.34
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	14	0.34
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	20	0.34
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	5	0.34
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	10	0.34
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	6	0.34
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	2	0.34
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	2	0.34
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	4	0.34
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	13	0.34
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	10	0.33
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	10	0.33
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	10	0.33
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	10	0.33
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	10	0.33
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	10	0.33
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	10	0.33
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	10	0.33
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	10	0.33
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	10	0.33
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	10	0.33
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	10	0.33
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	10	0.33
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	10	0.33
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	10	0.33
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	10	0.33
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	10	0.33
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	10	0.33
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	10	0.33
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	10	0.33
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	10	0.33
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	10	0.33
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	10	0.33
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	10	0.33
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	10	0.33
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	10	0.33
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	10	0.33
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	10	0.33
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	10	0.33
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	10	0.33
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	10	0.33
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	10	0.33
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	10	0.33
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	10	0.33
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	10	0.33
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	8	0.33
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	8	0.33
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	8	0.33
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	8	0.33
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	8	0.33
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	8	0.33
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	8	0.33
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	8	0.33
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	8	0.33
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	8	0.33
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	8	0.33
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	8	0.33
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	8	0.33
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	8	0.33
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	8	0.33
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	8	0.33
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	8	0.33
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	8	0.33
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	8	0.33
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	8	0.33
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	8	0.33
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	8	0.33
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	8	0.33
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	8	0.33
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	8	0.33
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	8	0.33
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	8	0.33
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	8	0.33
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	8	0.33
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	8	0.33
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	8	0.33
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	8	0.33
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	8	0.33
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	8	0.33
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	8	0.33
(1,404)	1:12:A:LEU:HD11	1:152:A:TRP:HE1	20	0.33
(1,404)	1:12:A:LEU:HD12	1:152:A:TRP:HE1	20	0.33
(1,404)	1:12:A:LEU:HD13	1:152:A:TRP:HE1	20	0.33
(1,404)	1:12:A:LEU:HD21	1:152:A:TRP:HE1	20	0.33
(1,404)	1:12:A:LEU:HD22	1:152:A:TRP:HE1	20	0.33
(1,404)	1:12:A:LEU:HD23	1:152:A:TRP:HE1	20	0.33
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	5	0.33
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	5	0.33
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	5	0.33
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	6	0.33
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	6	0.33
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	6	0.33
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	18	0.33
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	18	0.33
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	18	0.33
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	1	0.33
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	15	0.33
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	1	0.33
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	14	0.33
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	18	0.33
(1,238)	1:134:A:MET:H	1:136:A:THR:H	7	0.33
(1,237)	1:153:A:ASP:H	1:155:A:PHE:H	11	0.33
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	13	0.33
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	13	0.33
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	15	0.33
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	4	0.33
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	15	0.33
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	9	0.33
(1,158)	1:102:A:GLY:H	1:104:A:ILE:H	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	4	0.33
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	6	0.33
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	8	0.33
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	4	0.33
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	6	0.33
(1,136)	1:9:A:ASN:H	1:11:A:GLU:H	16	0.33
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	16	0.33
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	4	0.33
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	18	0.33
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	19	0.33
(1,63)	1:53:A:ALA:H	1:55:A:ARG:H	18	0.33
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	1	0.33
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	8	0.32
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	8	0.32
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	8	0.32
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	8	0.32
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	8	0.32
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	8	0.32
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	8	0.32
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	8	0.32
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	8	0.32
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	8	0.32
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	8	0.32
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	8	0.32
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	8	0.32
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	8	0.32
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	8	0.32
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	8	0.32
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	8	0.32
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	8	0.32
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	8	0.32
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	8	0.32
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	8	0.32
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	8	0.32
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	8	0.32
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	8	0.32
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	8	0.32
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	8	0.32
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	8	0.32
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	8	0.32
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	8	0.32
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	8	0.32
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	8	0.32
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	8	0.32
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	8	0.32
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	8	0.32
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	8	0.32
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	9	0.32
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	9	0.32
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	9	0.32
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	9	0.32
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	9	0.32
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	9	0.32
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	14	0.32
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	14	0.32
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	14	0.32
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	14	0.32
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	14	0.32
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	14	0.32
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	2	0.32
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	2	0.32
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	2	0.32
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	2	0.32
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	2	0.32
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	2	0.32
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	16	0.32
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	16	0.32
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	16	0.32
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	16	0.32
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	16	0.32
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	16	0.32
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	1	0.32
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	1	0.32
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	1	0.32
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	3	0.32
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	3	0.32
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	3	0.32
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	17	0.32
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	17	0.32
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	17	0.32
(1,394)	1:138:A:LEU:HD11	1:143:A:GLU:H	11	0.32
(1,394)	1:138:A:LEU:HD12	1:143:A:GLU:H	11	0.32
(1,394)	1:138:A:LEU:HD13	1:143:A:GLU:H	11	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	11	0.32
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	11	0.32
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	11	0.32
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	18	0.32
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	18	0.32
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	18	0.32
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	18	0.32
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	18	0.32
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	18	0.32
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	18	0.32
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	18	0.32
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	18	0.32
(1,342)	1:138:A:LEU:HD21	1:143:A:GLU:H	10	0.32
(1,342)	1:138:A:LEU:HD22	1:143:A:GLU:H	10	0.32
(1,342)	1:138:A:LEU:HD23	1:143:A:GLU:H	10	0.32
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	15	0.32
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	15	0.32
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	15	0.32
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	7	0.32
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	7	0.32
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	7	0.32
(1,297)	1:17:A:LEU:HD11	1:130:A:ILE:H	8	0.32
(1,297)	1:17:A:LEU:HD12	1:130:A:ILE:H	8	0.32
(1,297)	1:17:A:LEU:HD13	1:130:A:ILE:H	8	0.32
(1,297)	1:17:A:LEU:HD21	1:130:A:ILE:H	8	0.32
(1,297)	1:17:A:LEU:HD22	1:130:A:ILE:H	8	0.32
(1,297)	1:17:A:LEU:HD23	1:130:A:ILE:H	8	0.32
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD11	3	0.32
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD12	3	0.32
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD13	3	0.32
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	14	0.32
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	2	0.32
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	4	0.32
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	6	0.32
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	10	0.32
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	12	0.32
(1,238)	1:134:A:MET:H	1:136:A:THR:H	20	0.32
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	8	0.32
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	9	0.32
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	11	0.32
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	11	0.32
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:111:A:GLY:H	1:113:A:ALA:H	14	0.32
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	13	0.32
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	16	0.32
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	20	0.32
(1,158)	1:102:A:GLY:H	1:104:A:ILE:H	15	0.32
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	14	0.32
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	7	0.32
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	1	0.32
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	3	0.32
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	9	0.32
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	9	0.32
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	17	0.32
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	7	0.32
(1,85)	1:17:A:LEU:H	1:19:A:TYR:H	17	0.32
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	14	0.32
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	11	0.32
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	7	0.32
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	18	0.32
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	20	0.32
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	13	0.32
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	11	0.32
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	3	0.32
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	16	0.32
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	10	0.31
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	2	0.31
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	2	0.31
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	2	0.31
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	2	0.31
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	2	0.31
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	2	0.31
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	2	0.31
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	2	0.31
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	2	0.31
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	2	0.31
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	2	0.31
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	2	0.31
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	2	0.31
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	2	0.31
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	2	0.31
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	2	0.31
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	2	0.31
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	2	0.31
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	2	0.31
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	2	0.31
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	2	0.31
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	2	0.31
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	2	0.31
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	2	0.31
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	2	0.31
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	2	0.31
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	2	0.31
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	2	0.31
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	2	0.31
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	2	0.31
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	2	0.31
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	2	0.31
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	2	0.31
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	2	0.31
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	2	0.31
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	7	0.31
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	7	0.31
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	7	0.31
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	7	0.31
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	7	0.31
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	7	0.31
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	7	0.31
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	7	0.31
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	7	0.31
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	7	0.31
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	7	0.31
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	7	0.31
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	7	0.31
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	7	0.31
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	7	0.31
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	7	0.31
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	7	0.31
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	7	0.31
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	7	0.31
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	7	0.31
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	7	0.31
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	7	0.31
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	7	0.31
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	7	0.31
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	7	0.31
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	7	0.31
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	7	0.31
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	7	0.31
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	7	0.31
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	7	0.31
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	7	0.31
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	7	0.31
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	7	0.31
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	7	0.31
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	7	0.31
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	9	0.31
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	9	0.31
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	9	0.31
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	9	0.31
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	9	0.31
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	9	0.31
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	7	0.31
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	7	0.31
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	7	0.31
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	7	0.31
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	7	0.31
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	7	0.31
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	7	0.31
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	7	0.31
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	7	0.31
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	7	0.31
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	7	0.31
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	7	0.31
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	7	0.31
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	7	0.31
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	7	0.31
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	7	0.31
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	7	0.31
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	7	0.31
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	7	0.31
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	7	0.31
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	7	0.31
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	7	0.31
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	7	0.31
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	7	0.31
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	7	0.31
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	7	0.31
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	7	0.31
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	7	0.31
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	7	0.31
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	7	0.31
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	7	0.31
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	7	0.31
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	7	0.31
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	7	0.31
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	7	0.31
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	17	0.31
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	17	0.31
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	17	0.31
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	17	0.31
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	17	0.31
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	17	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	8	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	8	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	8	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	8	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	8	0.31
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	8	0.31
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG11	3	0.31
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG12	3	0.31
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG13	3	0.31
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG21	3	0.31
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG22	3	0.31
(1,442)	1:54:A:LEU:HD11	1:105:A:VAL:HG23	3	0.31
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG11	3	0.31
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG12	3	0.31
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG13	3	0.31
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG21	3	0.31
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG22	3	0.31
(1,442)	1:54:A:LEU:HD12	1:105:A:VAL:HG23	3	0.31
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG11	3	0.31
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG12	3	0.31
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG13	3	0.31
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG21	3	0.31
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG22	3	0.31
(1,442)	1:54:A:LEU:HD13	1:105:A:VAL:HG23	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG11	3	0.31
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG12	3	0.31
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG13	3	0.31
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG21	3	0.31
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG22	3	0.31
(1,442)	1:54:A:LEU:HD21	1:105:A:VAL:HG23	3	0.31
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG11	3	0.31
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG12	3	0.31
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG13	3	0.31
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG21	3	0.31
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG22	3	0.31
(1,442)	1:54:A:LEU:HD22	1:105:A:VAL:HG23	3	0.31
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG11	3	0.31
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG12	3	0.31
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG13	3	0.31
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG21	3	0.31
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG22	3	0.31
(1,442)	1:54:A:LEU:HD23	1:105:A:VAL:HG23	3	0.31
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD11	2	0.31
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD12	2	0.31
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD13	2	0.31
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD21	2	0.31
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD22	2	0.31
(1,438)	1:53:A:ALA:H	1:54:A:LEU:HD23	2	0.31
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	15	0.31
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	15	0.31
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	15	0.31
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	15	0.31
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	15	0.31
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	15	0.31
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	16	0.31
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	16	0.31
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	16	0.31
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	16	0.31
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	16	0.31
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	16	0.31
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	20	0.31
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	20	0.31
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	20	0.31
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	14	0.31
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	14	0.31
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	2	0.31
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	2	0.31
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	2	0.31
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	2	0.31
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	2	0.31
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	2	0.31
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	2	0.31
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	2	0.31
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	2	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD11	5	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD12	5	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD13	5	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD11	8	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD12	8	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD13	8	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD11	16	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD12	16	0.31
(1,287)	1:141:A:HIS:H	1:142:A:LEU:HD13	16	0.31
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	8	0.31
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	10	0.31
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	17	0.31
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	3	0.31
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	8	0.31
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	19	0.31
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	5	0.31
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	4	0.31
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	7	0.31
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	12	0.31
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	19	0.31
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	17	0.31
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	8	0.31
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	14	0.31
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	15	0.31
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	2	0.31
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	4	0.31
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	10	0.31
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	18	0.31
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	14	0.31
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	20	0.31
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	6	0.31
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	7	0.31
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	6	0.31
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	14	0.31
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	12	0.31
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	2	0.31
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	16	0.31
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	17	0.31
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	19	0.31
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	4	0.31
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	3	0.31
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	5	0.31
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	6	0.31
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	9	0.31
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	5	0.31
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	15	0.31
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	13	0.3
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	13	0.3
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	13	0.3
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	13	0.3
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	13	0.3
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	13	0.3
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	3	0.3
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	3	0.3
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	3	0.3
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	3	0.3
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	3	0.3
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	3	0.3
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	18	0.3
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	18	0.3
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	18	0.3
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	18	0.3
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	18	0.3
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	18	0.3
(1,394)	1:138:A:LEU:HD11	1:143:A:GLU:H	13	0.3
(1,394)	1:138:A:LEU:HD12	1:143:A:GLU:H	13	0.3
(1,394)	1:138:A:LEU:HD13	1:143:A:GLU:H	13	0.3
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	3	0.3
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	3	0.3
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	3	0.3
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	9	0.3
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	9	0.3
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	9	0.3
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	17	0.3
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	17	0.3
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	20	0.3
(1,249)	1:124:A:GLN:H	1:125:A:VAL:H	17	0.3
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	6	0.3
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	9	0.3
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	13	0.3
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	3	0.3
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	5	0.3
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	14	0.3
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	3	0.3
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	6	0.3
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	1	0.3
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	16	0.3
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	2	0.3
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	4	0.3
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	6	0.3
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	10	0.3
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	17	0.3
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	7	0.3
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	6	0.3
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	12	0.3
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	16	0.3
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	2	0.3
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	7	0.3
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	10	0.3
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	13	0.3
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	5	0.3
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	16	0.3
(1,40)	1:128:A:SER:H	1:130:A:ILE:H	3	0.3
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	15	0.3
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	19	0.3
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	20	0.3
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	14	0.29
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	1	0.29
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	1	0.29
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	1	0.29
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	1	0.29
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	1	0.29
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	1	0.29
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	1	0.29
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	1	0.29
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	1	0.29
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	1	0.29
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	1	0.29
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	1	0.29
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	1	0.29
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	1	0.29
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	1	0.29
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	1	0.29
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	1	0.29
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	1	0.29
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	1	0.29
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	1	0.29
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	1	0.29
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	1	0.29
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	1	0.29
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	1	0.29
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	1	0.29
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	1	0.29
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	1	0.29
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	1	0.29
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	1	0.29
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	1	0.29
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	1	0.29
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	1	0.29
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	1	0.29
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	1	0.29
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	1	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	13	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	13	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	13	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	13	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	13	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	13	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	13	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	13	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	13	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	13	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	13	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	13	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	13	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	13	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	13	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	13	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	13	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	13	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	13	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	13	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	13	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	13	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	13	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	13	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	13	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	13	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	13	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	13	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	13	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	13	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	13	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	13	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	13	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	13	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	13	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	14	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	14	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	14	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	14	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	14	0.29
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	14	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	14	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	14	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	14	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	14	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	14	0.29
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	14	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	14	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	14	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	14	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	14	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	14	0.29
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	14	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	14	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	14	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	14	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	14	0.29
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	14	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	14	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	14	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	14	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	14	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	14	0.29
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	14	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	14	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	14	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	14	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	14	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	14	0.29
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	14	0.29
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	5	0.29
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	5	0.29
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	5	0.29
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	5	0.29
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	5	0.29
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	5	0.29
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	14	0.29
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	14	0.29
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	14	0.29
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	14	0.29
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	14	0.29
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	14	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	1	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	1	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	1	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	1	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	1	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	1	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	10	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	10	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	10	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	10	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	10	0.29
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	10	0.29
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	17	0.29
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	17	0.29
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	17	0.29
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	17	0.29
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	17	0.29
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	11	0.29
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	11	0.29
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	11	0.29
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	11	0.29
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	11	0.29
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	11	0.29
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG11	20	0.29
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG12	20	0.29
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG13	20	0.29
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG21	20	0.29
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG22	20	0.29
(1,407)	1:13:A:VAL:HG11	1:14:A:VAL:HG23	20	0.29
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG11	20	0.29
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG12	20	0.29
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG13	20	0.29
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG21	20	0.29
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG22	20	0.29
(1,407)	1:13:A:VAL:HG12	1:14:A:VAL:HG23	20	0.29
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG11	20	0.29
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG12	20	0.29
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG13	20	0.29
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG21	20	0.29
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG22	20	0.29
(1,407)	1:13:A:VAL:HG13	1:14:A:VAL:HG23	20	0.29
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG11	20	0.29
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG12	20	0.29
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG13	20	0.29
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG21	20	0.29
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG22	20	0.29
(1,407)	1:13:A:VAL:HG21	1:14:A:VAL:HG23	20	0.29
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG11	20	0.29
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG12	20	0.29
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG13	20	0.29
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG21	20	0.29
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG22	20	0.29
(1,407)	1:13:A:VAL:HG22	1:14:A:VAL:HG23	20	0.29
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG11	20	0.29
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG12	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG13	20	0.29
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG21	20	0.29
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG22	20	0.29
(1,407)	1:13:A:VAL:HG23	1:14:A:VAL:HG23	20	0.29
(1,378)	1:17:A:LEU:HD11	1:113:A:ALA:H	8	0.29
(1,378)	1:17:A:LEU:HD12	1:113:A:ALA:H	8	0.29
(1,378)	1:17:A:LEU:HD13	1:113:A:ALA:H	8	0.29
(1,378)	1:17:A:LEU:HD21	1:113:A:ALA:H	8	0.29
(1,378)	1:17:A:LEU:HD22	1:113:A:ALA:H	8	0.29
(1,378)	1:17:A:LEU:HD23	1:113:A:ALA:H	8	0.29
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	6	0.29
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	6	0.29
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	6	0.29
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	13	0.29
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	13	0.29
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	13	0.29
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG11	7	0.29
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG12	7	0.29
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG13	7	0.29
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG21	7	0.29
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG22	7	0.29
(1,307)	1:24:A:LYS:H	1:116:A:VAL:HG23	7	0.29
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	2	0.29
(1,238)	1:134:A:MET:H	1:136:A:THR:H	1	0.29
(1,238)	1:134:A:MET:H	1:136:A:THR:H	15	0.29
(1,238)	1:134:A:MET:H	1:136:A:THR:H	16	0.29
(1,238)	1:134:A:MET:H	1:136:A:THR:H	18	0.29
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	1	0.29
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	14	0.29
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	7	0.29
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	15	0.29
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	16	0.29
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	9	0.29
(1,141)	1:140:A:ASP:H	1:142:A:LEU:H	5	0.29
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	12	0.29
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	17	0.29
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	8	0.29
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	5	0.29
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	12	0.29
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	1	0.29
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	6	0.29
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	6	0.29
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	18	0.29
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	11	0.29
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	20	0.29
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	14	0.29
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	2	0.29
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	5	0.29
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	8	0.29
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	9	0.29
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	6	0.29
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	13	0.29
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	7	0.29
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	13	0.29
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	15	0.29
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	15	0.29
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	19	0.29
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	9	0.29
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	20	0.29
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	20	0.28
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	20	0.28
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	20	0.28
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	20	0.28
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	20	0.28
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	20	0.28
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	8	0.28
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	8	0.28
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	8	0.28
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	8	0.28
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	8	0.28
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	8	0.28
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	8	0.28
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	8	0.28
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	8	0.28
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	8	0.28
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	8	0.28
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	8	0.28
(1,453)	1:72:A:LEU:HD11	1:95:A:PHE:H	11	0.28
(1,453)	1:72:A:LEU:HD12	1:95:A:PHE:H	11	0.28
(1,453)	1:72:A:LEU:HD13	1:95:A:PHE:H	11	0.28
(1,453)	1:72:A:LEU:HD21	1:95:A:PHE:H	11	0.28
(1,453)	1:72:A:LEU:HD22	1:95:A:PHE:H	11	0.28
(1,453)	1:72:A:LEU:HD23	1:95:A:PHE:H	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	1	0.28
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	1	0.28
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	1	0.28
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	1	0.28
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	1	0.28
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	1	0.28
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	1	0.28
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	1	0.28
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	1	0.28
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	1	0.28
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	1	0.28
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	1	0.28
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	6	0.28
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	6	0.28
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	6	0.28
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	6	0.28
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	6	0.28
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	6	0.28
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	12	0.28
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	12	0.28
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	12	0.28
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	12	0.28
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	12	0.28
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	12	0.28
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	20	0.28
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	20	0.28
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	20	0.28
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	20	0.28
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	20	0.28
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	20	0.28
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	9	0.28
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	9	0.28
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	9	0.28
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	9	0.28
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	9	0.28
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	9	0.28
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	4	0.28
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	4	0.28
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	4	0.28
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	11	0.28
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	11	0.28
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD11	17	0.28
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD12	17	0.28
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD13	17	0.28
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	5	0.28
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	5	0.28
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	5	0.28
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	5	0.28
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	5	0.28
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	5	0.28
(1,299)	1:78:A:ILE:HD11	1:119:A:VAL:H	20	0.28
(1,299)	1:78:A:ILE:HD12	1:119:A:VAL:H	20	0.28
(1,299)	1:78:A:ILE:HD13	1:119:A:VAL:H	20	0.28
(1,282)	1:12:A:LEU:HD11	1:51:A:LYS:H	9	0.28
(1,282)	1:12:A:LEU:HD12	1:51:A:LYS:H	9	0.28
(1,282)	1:12:A:LEU:HD13	1:51:A:LYS:H	9	0.28
(1,238)	1:134:A:MET:H	1:136:A:THR:H	3	0.28
(1,238)	1:134:A:MET:H	1:136:A:THR:H	9	0.28
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	10	0.28
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	3	0.28
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	8	0.28
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	16	0.28
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	7	0.28
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	8	0.28
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	1	0.28
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	9	0.28
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	19	0.28
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	5	0.28
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	9	0.28
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	19	0.28
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	18	0.28
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	16	0.28
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	11	0.28
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	9	0.28
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	12	0.28
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	4	0.28
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	1	0.28
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	11	0.28
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	20	0.28
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	2	0.28
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	3	0.28
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	6	0.28
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	12	0.28
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	3	0.28
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	5	0.28
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	16	0.28
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	8	0.27
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	8	0.27
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	8	0.27
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	8	0.27
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	8	0.27
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	8	0.27
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	9	0.27
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	9	0.27
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	9	0.27
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	9	0.27
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	9	0.27
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	9	0.27
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	16	0.27
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	16	0.27
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	16	0.27
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	16	0.27
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	16	0.27
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	16	0.27
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	19	0.27
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	19	0.27
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	19	0.27
(1,338)	1:12:A:LEU:HD21	1:51:A:LYS:H	16	0.27
(1,338)	1:12:A:LEU:HD22	1:51:A:LYS:H	16	0.27
(1,338)	1:12:A:LEU:HD23	1:51:A:LYS:H	16	0.27
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	2	0.27
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	2	0.27
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	2	0.27
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	5	0.27
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	17	0.27
(1,238)	1:134:A:MET:H	1:136:A:THR:H	8	0.27
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	12	0.27
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	11	0.27
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	16	0.27
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	14	0.27
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	13	0.27
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	13	0.27
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	18	0.27
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:154:A:THR:H	1:156:A:VAL:H	12	0.27
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	3	0.27
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	12	0.27
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	13	0.27
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	18	0.27
(1,139)	1:140:A:ASP:H	1:143:A:GLU:H	5	0.27
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	8	0.27
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	18	0.27
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	11	0.27
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	14	0.27
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	15	0.27
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	6	0.27
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	19	0.27
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	14	0.27
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	12	0.27
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	20	0.27
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	1	0.27
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	13	0.27
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	2	0.26
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	2	0.26
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	2	0.26
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	2	0.26
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	2	0.26
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	2	0.26
(2,1)	1:27:A:SER:H	1:32:A:SER:H	15	0.26
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	15	0.26
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	15	0.26
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	15	0.26
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	15	0.26
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	15	0.26
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	15	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	13	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	13	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	13	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	13	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	13	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	13	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	13	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	13	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	13	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	13	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	13	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	13	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	13	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	13	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	13	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	13	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	13	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	13	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	13	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	13	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	13	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	13	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	13	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	13	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	13	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	13	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	13	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	13	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	13	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	13	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	13	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	13	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	13	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	13	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	13	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	14	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	14	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	14	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	14	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	14	0.26
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	14	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	14	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	14	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	14	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	14	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	14	0.26
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	14	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	14	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	14	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	14	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	14	0.26
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	14	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	14	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	14	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	14	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	14	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	14	0.26
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	14	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	14	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	14	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	14	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	14	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	14	0.26
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	14	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	14	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	14	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	14	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	14	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	14	0.26
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	14	0.26
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	7	0.26
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	7	0.26
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	7	0.26
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	7	0.26
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	7	0.26
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	7	0.26
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	19	0.26
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	19	0.26
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	19	0.26
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	19	0.26
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	19	0.26
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	19	0.26
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	3	0.26
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	3	0.26
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	3	0.26
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	3	0.26
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	3	0.26
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	3	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	4	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	4	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	4	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	4	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	4	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	4	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	4	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	4	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	4	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	4	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	4	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	4	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	4	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	4	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	4	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	4	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	4	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	4	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	4	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	4	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	4	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	4	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	4	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	4	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	4	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	4	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	4	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	4	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	4	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	4	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	4	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	4	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	4	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	4	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	4	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	15	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	15	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	15	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	15	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	15	0.26
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	15	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	15	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	15	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	15	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	15	0.26
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	15	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	15	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	15	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	15	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	15	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	15	0.26
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	15	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	15	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	15	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	15	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	15	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	15	0.26
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	15	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	15	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	15	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	15	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	15	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	15	0.26
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	15	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	15	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	15	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	15	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	15	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	15	0.26
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	15	0.26
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	18	0.26
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	18	0.26
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	18	0.26
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD11	8	0.26
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD12	8	0.26
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD13	8	0.26
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG11	17	0.26
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG12	17	0.26
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG13	17	0.26
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG21	17	0.26
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG22	17	0.26
(1,324)	1:22:A:SER:H	1:116:A:VAL:HG23	17	0.26
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	15	0.26
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	15	0.26
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	15	0.26
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	4	0.26
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	11	0.26
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	2	0.26
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	6	0.26
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	4	0.26
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	7	0.26
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	4	0.26
(1,210)	1:101:A:TRP:H	1:103:A:ARG:H	4	0.26
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	11	0.26
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	5	0.26
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	11	0.26
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	12	0.26
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	19	0.26
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	4	0.26
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	9	0.26
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	12	0.26
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	15	0.26
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	20	0.26
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	9	0.26
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	5	0.26
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	8	0.26
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	10	0.26
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	20	0.26
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	10	0.26
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	18	0.26
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	3	0.26
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	8	0.26
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	12	0.26
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	13	0.26
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	15	0.26
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	18	0.26
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	4	0.26
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	5	0.26
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	8	0.26
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	4	0.26
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	11	0.26
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	20	0.26
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	19	0.25
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	2	0.25
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	2	0.25
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	2	0.25
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	2	0.25
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	2	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	3	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	3	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	3	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	3	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	3	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	3	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	3	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	3	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	3	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	3	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	3	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	3	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	3	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	3	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	3	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	3	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	3	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	3	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	3	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	3	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	3	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	3	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	3	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	3	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	3	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	3	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	3	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	3	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	3	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	3	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	3	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	3	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	3	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	3	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	3	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	3	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	8	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	8	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	8	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	8	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	8	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	8	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	8	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	8	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	8	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	8	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	8	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	8	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	8	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	8	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	8	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	8	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	8	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	8	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	8	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	8	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	8	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	8	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	8	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	8	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	8	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	8	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	8	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	8	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	8	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	8	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	8	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	8	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	8	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	8	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	8	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	16	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	16	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	16	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	16	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	16	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	16	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	16	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	16	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	16	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	16	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	16	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	16	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	16	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	16	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	16	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	16	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	16	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	16	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	16	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	16	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	16	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	16	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	16	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	16	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	16	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	16	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	16	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	16	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	16	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	16	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	16	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	16	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	16	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	16	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	16	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	20	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	20	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	20	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	20	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	20	0.25
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	20	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	20	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	20	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	20	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	20	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	20	0.25
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	20	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	20	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	20	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	20	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	20	0.25
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	20	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	20	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	20	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	20	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	20	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	20	0.25
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	20	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	20	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	20	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	20	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	20	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	20	0.25
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	20	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	20	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	20	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	20	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	20	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	20	0.25
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	20	0.25
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	3	0.25
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	3	0.25
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	3	0.25
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	3	0.25
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	3	0.25
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	3	0.25
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	17	0.25
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	17	0.25
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	17	0.25
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	17	0.25
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	17	0.25
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	17	0.25
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	18	0.25
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	18	0.25
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	18	0.25
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	18	0.25
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	18	0.25
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	18	0.25
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	6	0.25
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	6	0.25
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	6	0.25
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	6	0.25
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	6	0.25
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	8	0.25
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	8	0.25
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	8	0.25
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	8	0.25
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	8	0.25
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	8	0.25
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	9	0.25
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	9	0.25
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	9	0.25
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	9	0.25
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	9	0.25
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	9	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	5	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	5	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	5	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	5	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	5	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	5	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	5	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	5	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	5	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	5	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	5	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	5	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	5	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	5	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	5	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	5	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	5	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	5	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	5	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	5	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	5	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	5	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	5	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	5	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	5	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	5	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	5	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	5	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	5	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	5	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	5	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	5	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	5	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	5	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	5	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	13	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	13	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	13	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	13	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	13	0.25
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	13	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	13	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	13	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	13	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	13	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	13	0.25
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	13	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	13	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	13	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	13	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	13	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	13	0.25
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	13	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	13	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	13	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	13	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	13	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	13	0.25
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	13	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	13	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	13	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	13	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	13	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	13	0.25
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	13	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	13	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	13	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	13	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	13	0.25
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	13	0.25
(1,404)	1:12:A:LEU:HD11	1:152:A:TRP:HE1	3	0.25
(1,404)	1:12:A:LEU:HD12	1:152:A:TRP:HE1	3	0.25
(1,404)	1:12:A:LEU:HD13	1:152:A:TRP:HE1	3	0.25
(1,404)	1:12:A:LEU:HD21	1:152:A:TRP:HE1	3	0.25
(1,404)	1:12:A:LEU:HD22	1:152:A:TRP:HE1	3	0.25
(1,404)	1:12:A:LEU:HD23	1:152:A:TRP:HE1	3	0.25
(1,404)	1:12:A:LEU:HD11	1:152:A:TRP:HE1	5	0.25
(1,404)	1:12:A:LEU:HD12	1:152:A:TRP:HE1	5	0.25
(1,404)	1:12:A:LEU:HD13	1:152:A:TRP:HE1	5	0.25
(1,404)	1:12:A:LEU:HD21	1:152:A:TRP:HE1	5	0.25
(1,404)	1:12:A:LEU:HD22	1:152:A:TRP:HE1	5	0.25
(1,404)	1:12:A:LEU:HD23	1:152:A:TRP:HE1	5	0.25
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	12	0.25
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	12	0.25
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	12	0.25
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	9	0.25
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	9	0.25
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	9	0.25
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	14	0.25
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	14	0.25
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	14	0.25
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	15	0.25
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	17	0.25
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	20	0.25
(1,239)	1:12:A:LEU:H	1:14:A:VAL:H	11	0.25
(1,238)	1:134:A:MET:H	1:136:A:THR:H	2	0.25
(1,238)	1:134:A:MET:H	1:136:A:THR:H	5	0.25
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	11	0.25
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	2	0.25
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	3	0.25
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	9	0.25
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	18	0.25
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	6	0.25
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	19	0.25
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	15	0.25
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	2	0.25
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	14	0.25
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	7	0.25
(1,177)	1:156:A:VAL:H	1:159:A:TYR:H	12	0.25
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	16	0.25
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	1	0.25
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	4	0.25
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	10	0.25
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	15	0.25
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	16	0.25
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	3	0.25
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	15	0.25
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	3	0.25
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	8	0.25
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	6	0.25
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	13	0.25
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	19	0.25
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	15	0.25
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	20	0.25
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	10	0.25
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	5	0.25
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	16	0.25
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	3	0.25
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	9	0.25
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	4	0.25
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	7	0.25
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	10	0.25
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	12	0.25
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	17	0.25
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	10	0.25
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	7	0.25
(1,16)	1:89:A:GLN:H	1:92:A:ASN:H	10	0.25
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	3	0.25
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	8	0.25
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	12	0.25
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	4	0.25
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	17	0.25
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	10	0.24
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	10	0.24
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	10	0.24
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	10	0.24
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	10	0.24
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	10	0.24
(1,505)	1:138:A:LEU:HD11	1:152:A:TRP:HE1	14	0.24
(1,505)	1:138:A:LEU:HD12	1:152:A:TRP:HE1	14	0.24
(1,505)	1:138:A:LEU:HD13	1:152:A:TRP:HE1	14	0.24
(1,505)	1:138:A:LEU:HD21	1:152:A:TRP:HE1	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:138:A:LEU:HD22	1:152:A:TRP:HE1	14	0.24
(1,505)	1:138:A:LEU:HD23	1:152:A:TRP:HE1	14	0.24
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD11	17	0.24
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD12	17	0.24
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD13	17	0.24
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD21	17	0.24
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD22	17	0.24
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD23	17	0.24
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	9	0.24
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	9	0.24
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	9	0.24
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	9	0.24
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	9	0.24
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	9	0.24
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	15	0.24
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	15	0.24
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	15	0.24
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	15	0.24
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	15	0.24
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	15	0.24
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	9	0.24
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	9	0.24
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	9	0.24
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	9	0.24
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	9	0.24
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	9	0.24
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	6	0.24
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	6	0.24
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	6	0.24
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	6	0.24
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	6	0.24
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	6	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	14	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	14	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	14	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	14	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	14	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	14	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	14	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	14	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	14	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	14	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	14	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	14	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	14	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	14	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	14	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	14	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	14	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	14	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	14	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	14	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	14	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	14	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	14	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	14	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	14	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	14	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	14	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	14	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	14	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	14	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	14	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	14	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	14	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	14	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	14	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	16	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	16	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	16	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	16	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	16	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	16	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	16	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	16	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	16	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	16	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	16	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	16	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	16	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	16	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	16	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	16	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	16	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	16	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	16	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	16	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	16	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	16	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	16	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	16	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	16	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	16	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	16	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	16	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	16	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	16	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	16	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	16	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	16	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	16	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	16	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	18	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	18	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	18	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	18	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	18	0.24
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	18	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	18	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	18	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	18	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	18	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	18	0.24
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	18	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	18	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	18	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	18	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	18	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	18	0.24
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	18	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	18	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	18	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	18	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	18	0.24
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	18	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	18	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	18	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	18	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	18	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	18	0.24
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	18	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	18	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	18	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	18	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	18	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	18	0.24
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	18	0.24
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	6	0.24
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	6	0.24
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	6	0.24
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD11	10	0.24
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD12	10	0.24
(1,288)	1:16:A:PHE:H	1:54:A:LEU:HD13	10	0.24
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	2	0.24
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	5	0.24
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	9	0.24
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	18	0.24
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	16	0.24
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	7	0.24
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	13	0.24
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	20	0.24
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	13	0.24
(1,214)	1:26:A:TYR:H	1:27:A:SER:H	15	0.24
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	17	0.24
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	7	0.24
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	2	0.24
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	1	0.24
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	3	0.24
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	4	0.24
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	5	0.24
(1,158)	1:102:A:GLY:H	1:104:A:ILE:H	13	0.24
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	3	0.24
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	6	0.24
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	7	0.24
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	11	0.24
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	7	0.24
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	13	0.24
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	2	0.24
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	6	0.24
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	8	0.24
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	13	0.24
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	18	0.24
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	20	0.24
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	2	0.24
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	15	0.24
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	4	0.24
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	13	0.24
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	14	0.24
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	14	0.24
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	4	0.24
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	16	0.24
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	2	0.24
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	15	0.24
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	11	0.24
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	12	0.24
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	15	0.24
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	11	0.24
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	14	0.24
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	1	0.24
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	2	0.24
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	6	0.24
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	11	0.24
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD11	17	0.23
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD12	17	0.23
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD13	17	0.23
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD21	17	0.23
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD22	17	0.23
(2,10)	1:116:A:VAL:H	1:126:A:LEU:HD23	17	0.23
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	20	0.23
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	20	0.23
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	20	0.23
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	20	0.23
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	20	0.23
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	20	0.23
(1,511)	1:158:A:LEU:HD11	1:160:A:GLY:H	13	0.23
(1,511)	1:158:A:LEU:HD12	1:160:A:GLY:H	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:158:A:LEU:HD13	1:160:A:GLY:H	13	0.23
(1,511)	1:158:A:LEU:HD21	1:160:A:GLY:H	13	0.23
(1,511)	1:158:A:LEU:HD22	1:160:A:GLY:H	13	0.23
(1,511)	1:158:A:LEU:HD23	1:160:A:GLY:H	13	0.23
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD11	3	0.23
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD12	3	0.23
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD13	3	0.23
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD21	3	0.23
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD22	3	0.23
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD23	3	0.23
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	5	0.23
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	5	0.23
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	5	0.23
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	5	0.23
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	5	0.23
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	5	0.23
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	5	0.23
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	5	0.23
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	5	0.23
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	5	0.23
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	5	0.23
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	5	0.23
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	5	0.23
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	5	0.23
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	5	0.23
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	5	0.23
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	5	0.23
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	5	0.23
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	5	0.23
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	5	0.23
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	5	0.23
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	5	0.23
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	5	0.23
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	5	0.23
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	5	0.23
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	5	0.23
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	5	0.23
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	5	0.23
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	5	0.23
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	5	0.23
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	5	0.23
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	5	0.23
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	5	0.23
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	5	0.23
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	5	0.23
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	5	0.23
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	5	0.23
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	5	0.23
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	5	0.23
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	5	0.23
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	5	0.23
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	5	0.23
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	5	0.23
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	5	0.23
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	5	0.23
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	5	0.23
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	5	0.23
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	5	0.23
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	5	0.23
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	5	0.23
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	5	0.23
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	5	0.23
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	5	0.23
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	5	0.23
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	5	0.23
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	5	0.23
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	5	0.23
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	5	0.23
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	5	0.23
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	5	0.23
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	5	0.23
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	5	0.23
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	5	0.23
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	5	0.23
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	5	0.23
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	5	0.23
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	5	0.23
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	5	0.23
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	5	0.23
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	5	0.23
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	5	0.23
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	20	0.23
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	20	0.23
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	20	0.23
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	20	0.23
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	20	0.23
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	12	0.23
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	12	0.23
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	12	0.23
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	12	0.23
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	12	0.23
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	12	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	6	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	6	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	6	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	6	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	6	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	6	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	14	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	14	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	14	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	14	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	14	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	14	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	16	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	16	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	16	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	16	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	16	0.23
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	16	0.23
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	16	0.23
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	16	0.23
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	16	0.23
(1,377)	1:17:A:LEU:HD11	1:111:A:GLY:H	12	0.23
(1,377)	1:17:A:LEU:HD12	1:111:A:GLY:H	12	0.23
(1,377)	1:17:A:LEU:HD13	1:111:A:GLY:H	12	0.23
(1,377)	1:17:A:LEU:HD21	1:111:A:GLY:H	12	0.23
(1,377)	1:17:A:LEU:HD22	1:111:A:GLY:H	12	0.23
(1,377)	1:17:A:LEU:HD23	1:111:A:GLY:H	12	0.23
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	15	0.23
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	15	0.23
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	15	0.23
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	8	0.23
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	3	0.23
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	16	0.23
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	10	0.23
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	18	0.23
(1,241)	1:12:A:LEU:H	1:13:A:VAL:H	19	0.23
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	15	0.23
(1,224)	1:52:A:GLN:H	1:54:A:LEU:H	10	0.23
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	2	0.23
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	2	0.23
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	14	0.23
(1,212)	1:99:A:VAL:H	1:102:A:GLY:H	11	0.23
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	1	0.23
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	13	0.23
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	19	0.23
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	4	0.23
(1,195)	1:148:A:GLU:H	1:149:A:ASN:H	8	0.23
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	7	0.23
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	11	0.23
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	16	0.23
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	19	0.23
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	14	0.23
(1,170)	1:40:A:GLU:H	1:41:A:ALA:H	3	0.23
(1,158)	1:102:A:GLY:H	1:104:A:ILE:H	11	0.23
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	12	0.23
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	14	0.23
(1,150)	1:126:A:LEU:H	1:129:A:ARG:H	10	0.23
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	20	0.23
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	11	0.23
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	1	0.23
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	2	0.23
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	5	0.23
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	1	0.23
(1,100)	1:155:A:PHE:H	1:157:A:GLU:H	10	0.23
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	14	0.23
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	15	0.23
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	8	0.23
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	1	0.23
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	2	0.23
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	20	0.23
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	20	0.23
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	3	0.23
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	10	0.23
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	11	0.23
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	2	0.23
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	9	0.23
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	18	0.23
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	12	0.23
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	14	0.23
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	1	0.22
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	1	0.22
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	1	0.22
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	1	0.22
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	1	0.22
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	1	0.22
(1,505)	1:138:A:LEU:HD11	1:152:A:TRP:HE1	5	0.22
(1,505)	1:138:A:LEU:HD12	1:152:A:TRP:HE1	5	0.22
(1,505)	1:138:A:LEU:HD13	1:152:A:TRP:HE1	5	0.22
(1,505)	1:138:A:LEU:HD21	1:152:A:TRP:HE1	5	0.22
(1,505)	1:138:A:LEU:HD22	1:152:A:TRP:HE1	5	0.22
(1,505)	1:138:A:LEU:HD23	1:152:A:TRP:HE1	5	0.22
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	19	0.22
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	19	0.22
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	19	0.22
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	19	0.22
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	19	0.22
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	19	0.22
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	19	0.22
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	19	0.22
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	19	0.22
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	19	0.22
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	19	0.22
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	19	0.22
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	19	0.22
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	19	0.22
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	19	0.22
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	19	0.22
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	19	0.22
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	19	0.22
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	19	0.22
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	19	0.22
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	19	0.22
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	19	0.22
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	19	0.22
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	19	0.22
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	19	0.22
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	19	0.22
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	19	0.22
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	19	0.22
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	19	0.22
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	19	0.22
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	19	0.22
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	19	0.22
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	19	0.22
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	19	0.22
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	19	0.22
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD11	4	0.22
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD12	4	0.22
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD13	4	0.22
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD21	4	0.22
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD22	4	0.22
(1,415)	1:14:A:VAL:H	1:54:A:LEU:HD23	4	0.22
(1,394)	1:138:A:LEU:HD11	1:143:A:GLU:H	9	0.22
(1,394)	1:138:A:LEU:HD12	1:143:A:GLU:H	9	0.22
(1,394)	1:138:A:LEU:HD13	1:143:A:GLU:H	9	0.22
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	14	0.22
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	14	0.22
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	14	0.22
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	14	0.22
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	14	0.22
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	14	0.22
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	1	0.22
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	1	0.22
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	1	0.22
(1,373)	1:13:A:VAL:HG21	1:136:A:THR:H	10	0.22
(1,373)	1:13:A:VAL:HG22	1:136:A:THR:H	10	0.22
(1,373)	1:13:A:VAL:HG23	1:136:A:THR:H	10	0.22
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	2	0.22
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	2	0.22
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	2	0.22
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	13	0.22
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	15	0.22
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	1	0.22
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	14	0.22
(1,238)	1:134:A:MET:H	1:136:A:THR:H	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	16	0.22
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	18	0.22
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	19	0.22
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	7	0.22
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	12	0.22
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	14	0.22
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	14	0.22
(1,214)	1:26:A:TYR:H	1:27:A:SER:H	8	0.22
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	9	0.22
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	13	0.22
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	10	0.22
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	2	0.22
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	5	0.22
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	6	0.22
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	8	0.22
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	4	0.22
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	5	0.22
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	13	0.22
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	20	0.22
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	6	0.22
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	2	0.22
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	7	0.22
(1,154)	1:96:A:ARG:H	1:98:A:GLY:H	5	0.22
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	8	0.22
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	18	0.22
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	13	0.22
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	20	0.22
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	12	0.22
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	4	0.22
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	3	0.22
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	11	0.22
(1,105)	1:33:A:ASP:H	1:35:A:GLU:H	13	0.22
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	2	0.22
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	17	0.22
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	20	0.22
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	7	0.22
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	7	0.22
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	4	0.22
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	12	0.22
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	20	0.22
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	13	0.22
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	8	0.22
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	20	0.22
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	19	0.22
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	20	0.22
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	19	0.22
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	5	0.22
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	16	0.22
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	19	0.22
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	19	0.22
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	2	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	2	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	2	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	2	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	2	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	2	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	2	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	2	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	2	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	2	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	2	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	2	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	2	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	2	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	2	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	2	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	2	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	2	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	2	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	2	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	2	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	2	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	2	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	2	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	2	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	2	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	2	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	2	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	2	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	2	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	2	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	2	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	2	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	2	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	2	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	4	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	4	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	4	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	4	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	4	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	4	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	4	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	4	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	4	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	4	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	4	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	4	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	4	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	4	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	4	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	4	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	4	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	4	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	4	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	4	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	4	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	4	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	4	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	4	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	4	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	4	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	4	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	4	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	4	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	4	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	4	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	4	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	4	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	4	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	4	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	4	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	12	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	12	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	12	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	12	0.21
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	12	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	12	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	12	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	12	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	12	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	12	0.21
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	12	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	12	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	12	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	12	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	12	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	12	0.21
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	12	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	12	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	12	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	12	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	12	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	12	0.21
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	12	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	12	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	12	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	12	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	12	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	12	0.21
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	12	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	12	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	12	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	12	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	12	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	12	0.21
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	12	0.21
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	6	0.21
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	6	0.21
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	6	0.21
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	6	0.21
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	6	0.21
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	6	0.21
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG11	16	0.21
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG12	16	0.21
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG13	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG21	16	0.21
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG22	16	0.21
(1,444)	1:60:A:GLU:H	1:105:A:VAL:HG23	16	0.21
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	10	0.21
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	10	0.21
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	10	0.21
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	10	0.21
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	10	0.21
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	10	0.21
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	18	0.21
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	18	0.21
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	18	0.21
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	18	0.21
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	18	0.21
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	18	0.21
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	7	0.21
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	7	0.21
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	7	0.21
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD21	13	0.21
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD22	13	0.21
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD23	13	0.21
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD21	13	0.21
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD22	13	0.21
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD23	13	0.21
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD21	13	0.21
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD22	13	0.21
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD23	13	0.21
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD21	1	0.21
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD22	1	0.21
(1,358)	1:141:A:HIS:H	1:142:A:LEU:HD23	1	0.21
(1,338)	1:12:A:LEU:HD21	1:51:A:LYS:H	15	0.21
(1,338)	1:12:A:LEU:HD22	1:51:A:LYS:H	15	0.21
(1,338)	1:12:A:LEU:HD23	1:51:A:LYS:H	15	0.21
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD11	18	0.21
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD12	18	0.21
(1,314)	1:116:A:VAL:H	1:130:A:ILE:HD13	18	0.21
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	1	0.21
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	1	0.21
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	1	0.21
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	1	0.21
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	7	0.21
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	1	0.21
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	9	0.21
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	15	0.21
(1,212)	1:99:A:VAL:H	1:102:A:GLY:H	9	0.21
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	2	0.21
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	18	0.21
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	6	0.21
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	16	0.21
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	17	0.21
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	10	0.21
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	18	0.21
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	15	0.21
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	17	0.21
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	8	0.21
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	9	0.21
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	20	0.21
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	10	0.21
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	12	0.21
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	4	0.21
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	19	0.21
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	7	0.21
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	6	0.21
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	15	0.21
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	9	0.21
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	4	0.21
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	17	0.21
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	1	0.21
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	5	0.21
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	16	0.21
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	5	0.21
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	14	0.21
(1,79)	1:27:A:SER:H	1:30:A:GLN:H	5	0.21
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	1	0.21
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	6	0.21
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	1	0.21
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	7	0.21
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	11	0.21
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	17	0.21
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	14	0.21
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	7	0.21
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	8	0.21
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	17	0.21
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	18	0.21
(1,44)	1:60:A:GLU:H	1:62:A:GLU:H	4	0.21
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	7	0.21
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	17	0.21
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	3	0.21
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	18	0.21
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	1	0.21
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	4	0.21
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	18	0.21
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD11	10	0.2
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD12	10	0.2
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD13	10	0.2
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD21	10	0.2
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD22	10	0.2
(1,492)	1:125:A:VAL:HG11	1:126:A:LEU:HD23	10	0.2
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD11	10	0.2
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD12	10	0.2
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD13	10	0.2
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD21	10	0.2
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD22	10	0.2
(1,492)	1:125:A:VAL:HG12	1:126:A:LEU:HD23	10	0.2
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD11	10	0.2
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD12	10	0.2
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD13	10	0.2
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD21	10	0.2
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD22	10	0.2
(1,492)	1:125:A:VAL:HG13	1:126:A:LEU:HD23	10	0.2
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD11	10	0.2
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD12	10	0.2
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD13	10	0.2
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD21	10	0.2
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD22	10	0.2
(1,492)	1:125:A:VAL:HG21	1:126:A:LEU:HD23	10	0.2
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD11	10	0.2
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD12	10	0.2
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD13	10	0.2
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD21	10	0.2
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD22	10	0.2
(1,492)	1:125:A:VAL:HG22	1:126:A:LEU:HD23	10	0.2
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD11	10	0.2
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD12	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD13	10	0.2
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD21	10	0.2
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD22	10	0.2
(1,492)	1:125:A:VAL:HG23	1:126:A:LEU:HD23	10	0.2
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	18	0.2
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	18	0.2
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	18	0.2
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	18	0.2
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	18	0.2
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	18	0.2
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	19	0.2
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	19	0.2
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	19	0.2
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	19	0.2
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	19	0.2
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	19	0.2
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	19	0.2
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	19	0.2
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	19	0.2
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	19	0.2
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	19	0.2
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	19	0.2
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	19	0.2
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	19	0.2
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	19	0.2
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	19	0.2
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	19	0.2
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	19	0.2
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	19	0.2
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	19	0.2
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	19	0.2
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	19	0.2
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	19	0.2
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	19	0.2
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	19	0.2
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	19	0.2
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	19	0.2
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	19	0.2
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	19	0.2
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	19	0.2
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	19	0.2
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	19	0.2
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	19	0.2
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	19	0.2
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	19	0.2
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	19	0.2
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	19	0.2
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	19	0.2
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	19	0.2
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	19	0.2
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	19	0.2
(1,449)	1:72:A:LEU:HD11	1:91:A:VAL:H	10	0.2
(1,449)	1:72:A:LEU:HD12	1:91:A:VAL:H	10	0.2
(1,449)	1:72:A:LEU:HD13	1:91:A:VAL:H	10	0.2
(1,449)	1:72:A:LEU:HD21	1:91:A:VAL:H	10	0.2
(1,449)	1:72:A:LEU:HD22	1:91:A:VAL:H	10	0.2
(1,449)	1:72:A:LEU:HD23	1:91:A:VAL:H	10	0.2
(1,448)	1:72:A:LEU:HD11	1:90:A:VAL:H	16	0.2
(1,448)	1:72:A:LEU:HD12	1:90:A:VAL:H	16	0.2
(1,448)	1:72:A:LEU:HD13	1:90:A:VAL:H	16	0.2
(1,448)	1:72:A:LEU:HD21	1:90:A:VAL:H	16	0.2
(1,448)	1:72:A:LEU:HD22	1:90:A:VAL:H	16	0.2
(1,448)	1:72:A:LEU:HD23	1:90:A:VAL:H	16	0.2
(1,434)	1:50:A:VAL:HG11	1:152:A:TRP:H	1	0.2
(1,434)	1:50:A:VAL:HG12	1:152:A:TRP:H	1	0.2
(1,434)	1:50:A:VAL:HG13	1:152:A:TRP:H	1	0.2
(1,434)	1:50:A:VAL:HG21	1:152:A:TRP:H	1	0.2
(1,434)	1:50:A:VAL:HG22	1:152:A:TRP:H	1	0.2
(1,434)	1:50:A:VAL:HG23	1:152:A:TRP:H	1	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	6	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	6	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	6	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	6	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	6	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	6	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	6	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	6	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	6	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	6	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	6	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	6	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	6	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	6	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	6	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	6	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	6	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	6	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	6	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	6	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	6	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	6	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	6	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	6	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	6	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	6	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	6	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	6	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	6	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	6	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	6	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	6	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	6	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	6	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	6	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	19	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	19	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	19	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	19	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	19	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	19	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	19	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	19	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	19	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	19	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	19	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	19	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	19	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	19	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	19	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	19	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	19	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	19	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	19	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	19	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	19	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	19	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	19	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	19	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	19	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	19	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	19	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	19	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	19	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	19	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	19	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	19	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	19	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	19	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	19	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	20	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	20	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	20	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	20	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	20	0.2
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	20	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	20	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	20	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	20	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	20	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	20	0.2
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	20	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	20	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	20	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	20	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	20	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	20	0.2
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	20	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	20	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	20	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	20	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	20	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	20	0.2
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	20	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	20	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	20	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	20	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	20	0.2
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	20	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	20	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	20	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	20	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	20	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	20	0.2
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	20	0.2
(1,425)	1:21:A:LEU:HD11	1:119:A:VAL:H	16	0.2
(1,425)	1:21:A:LEU:HD12	1:119:A:VAL:H	16	0.2
(1,425)	1:21:A:LEU:HD13	1:119:A:VAL:H	16	0.2
(1,425)	1:21:A:LEU:HD21	1:119:A:VAL:H	16	0.2
(1,425)	1:21:A:LEU:HD22	1:119:A:VAL:H	16	0.2
(1,425)	1:21:A:LEU:HD23	1:119:A:VAL:H	16	0.2
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	3	0.2
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	3	0.2
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	3	0.2
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	11	0.2
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	11	0.2
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	11	0.2
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	14	0.2
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	14	0.2
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	14	0.2
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	15	0.2
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	15	0.2
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	15	0.2
(1,394)	1:138:A:LEU:HD11	1:143:A:GLU:H	19	0.2
(1,394)	1:138:A:LEU:HD12	1:143:A:GLU:H	19	0.2
(1,394)	1:138:A:LEU:HD13	1:143:A:GLU:H	19	0.2
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	8	0.2
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	8	0.2
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	8	0.2
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	2	0.2
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	9	0.2
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	1	0.2
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	12	0.2
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	14	0.2
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	2	0.2
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	3	0.2
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	9	0.2
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	13	0.2
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	3	0.2
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	20	0.2
(1,234)	1:116:A:VAL:H	1:117:A:GLU:H	17	0.2
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	9	0.2
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	10	0.2
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	4	0.2
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	3	0.2
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	12	0.2
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	5	0.2
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	8	0.2
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	10	0.2
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	17	0.2
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	15	0.2
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	12	0.2
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	3	0.2
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	14	0.2
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	19	0.2
(1,152)	1:127:A:VAL:H	1:129:A:ARG:H	17	0.2
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	5	0.2
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	19	0.2
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	2	0.2
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	8	0.2
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	3	0.2
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	10	0.2
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	14	0.2
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	3	0.2
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	5	0.2
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	19	0.2
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	4	0.2
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	13	0.2
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	15	0.2
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	6	0.2
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	11	0.2
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	18	0.2
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	2	0.2
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	11	0.2
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	3	0.2
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	14	0.2
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	19	0.2
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	3	0.2
(1,21)	1:43:A:GLU:H	1:44:A:GLY:H	19	0.2
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	1	0.2
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	17	0.2
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	6	0.2
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	10	0.2
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	6	0.2
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	8	0.2
(2,6)	1:78:A:ILE:HD11	1:128:A:SER:H	8	0.19
(2,6)	1:78:A:ILE:HD12	1:128:A:SER:H	8	0.19
(2,6)	1:78:A:ILE:HD13	1:128:A:SER:H	8	0.19
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG11	17	0.19
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG12	17	0.19
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG13	17	0.19
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG21	17	0.19
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG22	17	0.19
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG23	17	0.19
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG11	17	0.19
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG12	17	0.19
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG13	17	0.19
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG21	17	0.19
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG22	17	0.19
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG23	17	0.19
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG11	17	0.19
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG12	17	0.19
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG13	17	0.19
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG21	17	0.19
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG22	17	0.19
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG23	17	0.19
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG11	17	0.19
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG12	17	0.19
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG13	17	0.19
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG21	17	0.19
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG22	17	0.19
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG23	17	0.19
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG11	17	0.19
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG12	17	0.19
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG13	17	0.19
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG21	17	0.19
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG22	17	0.19
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG23	17	0.19
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG11	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG12	17	0.19
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG13	17	0.19
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG21	17	0.19
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG22	17	0.19
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG23	17	0.19
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD11	16	0.19
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD12	16	0.19
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD13	16	0.19
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD21	16	0.19
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD22	16	0.19
(1,470)	1:99:A:VAL:H	1:142:A:LEU:HD23	16	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	10	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	10	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	10	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	10	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	10	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	10	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	10	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	10	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	10	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	10	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	10	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	10	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	10	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	10	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	10	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	10	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	10	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	10	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	10	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	10	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	10	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	10	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	10	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	10	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	10	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	10	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	10	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	10	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	10	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	10	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	10	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	10	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	10	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	10	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	10	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	15	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	15	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	15	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	15	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	15	0.19
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	15	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	15	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	15	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	15	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	15	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	15	0.19
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	15	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	15	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	15	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	15	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	15	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	15	0.19
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	15	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	15	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	15	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	15	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	15	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	15	0.19
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	15	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	15	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	15	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	15	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	15	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	15	0.19
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	15	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	15	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	15	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	15	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	15	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	15	0.19
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	15	0.19
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	13	0.19
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	13	0.19
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	13	0.19
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	13	0.19
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	13	0.19
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	14	0.19
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	14	0.19
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	14	0.19
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	14	0.19
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	14	0.19
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	14	0.19
(1,448)	1:72:A:LEU:HD11	1:90:A:VAL:H	15	0.19
(1,448)	1:72:A:LEU:HD12	1:90:A:VAL:H	15	0.19
(1,448)	1:72:A:LEU:HD13	1:90:A:VAL:H	15	0.19
(1,448)	1:72:A:LEU:HD21	1:90:A:VAL:H	15	0.19
(1,448)	1:72:A:LEU:HD22	1:90:A:VAL:H	15	0.19
(1,448)	1:72:A:LEU:HD23	1:90:A:VAL:H	15	0.19
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	11	0.19
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	11	0.19
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	11	0.19
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	11	0.19
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	11	0.19
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	11	0.19
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	10	0.19
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	10	0.19
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	10	0.19
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	10	0.19
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	10	0.19
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	10	0.19
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	14	0.19
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	14	0.19
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	14	0.19
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	14	0.19
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	14	0.19
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	14	0.19
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	18	0.19
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	18	0.19
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	18	0.19
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	20	0.19
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	20	0.19
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	20	0.19
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD11	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD12	17	0.19
(1,364)	1:99:A:VAL:HG21	1:104:A:ILE:HD13	17	0.19
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD11	17	0.19
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD12	17	0.19
(1,364)	1:99:A:VAL:HG22	1:104:A:ILE:HD13	17	0.19
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD11	17	0.19
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD12	17	0.19
(1,364)	1:99:A:VAL:HG23	1:104:A:ILE:HD13	17	0.19
(1,362)	1:72:A:LEU:HD21	1:110:A:PHE:H	18	0.19
(1,362)	1:72:A:LEU:HD22	1:110:A:PHE:H	18	0.19
(1,362)	1:72:A:LEU:HD23	1:110:A:PHE:H	18	0.19
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	6	0.19
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	6	0.19
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	6	0.19
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	5	0.19
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	5	0.19
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	5	0.19
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	18	0.19
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	18	0.19
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	18	0.19
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	14	0.19
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	12	0.19
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	18	0.19
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	3	0.19
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	8	0.19
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	17	0.19
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	19	0.19
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	8	0.19
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	6	0.19
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	8	0.19
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	19	0.19
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	4	0.19
(1,221)	1:125:A:VAL:H	1:127:A:VAL:H	17	0.19
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	6	0.19
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	10	0.19
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	11	0.19
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	20	0.19
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	4	0.19
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	12	0.19
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	20	0.19
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	15	0.19
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	3	0.19
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	4	0.19
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	16	0.19
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	9	0.19
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	12	0.19
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	13	0.19
(1,152)	1:127:A:VAL:H	1:129:A:ARG:H	20	0.19
(1,150)	1:126:A:LEU:H	1:129:A:ARG:H	19	0.19
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	13	0.19
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	20	0.19
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	14	0.19
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	20	0.19
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	11	0.19
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	19	0.19
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	1	0.19
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	6	0.19
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	10	0.19
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	13	0.19
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	18	0.19
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	4	0.19
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	1	0.19
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	2	0.19
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	3	0.19
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	16	0.19
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	1	0.19
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	5	0.19
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	6	0.19
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	15	0.19
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	6	0.19
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	18	0.19
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	5	0.19
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	2	0.19
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	7	0.19
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	7	0.19
(1,72)	1:88:A:GLU:H	1:91:A:VAL:H	10	0.19
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	5	0.19
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	13	0.19
(1,60)	1:13:A:VAL:H	1:16:A:PHE:H	17	0.19
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	20	0.19
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	18	0.19
(1,47)	1:57:A:ALA:H	1:59:A:ASP:H	17	0.19
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	19	0.19
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	12	0.19
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	6	0.19
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	10	0.19
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	12	0.19
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	8	0.19
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	10	0.19
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	17	0.19
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	1	0.19
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	2	0.19
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD11	5	0.18
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD12	5	0.18
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD13	5	0.18
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD21	5	0.18
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD22	5	0.18
(2,9)	1:101:A:TRP:H	1:142:A:LEU:HD23	5	0.18
(2,6)	1:78:A:ILE:HD11	1:128:A:SER:H	17	0.18
(2,6)	1:78:A:ILE:HD12	1:128:A:SER:H	17	0.18
(2,6)	1:78:A:ILE:HD13	1:128:A:SER:H	17	0.18
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	15	0.18
(1,505)	1:138:A:LEU:HD11	1:152:A:TRP:HE1	13	0.18
(1,505)	1:138:A:LEU:HD12	1:152:A:TRP:HE1	13	0.18
(1,505)	1:138:A:LEU:HD13	1:152:A:TRP:HE1	13	0.18
(1,505)	1:138:A:LEU:HD21	1:152:A:TRP:HE1	13	0.18
(1,505)	1:138:A:LEU:HD22	1:152:A:TRP:HE1	13	0.18
(1,505)	1:138:A:LEU:HD23	1:152:A:TRP:HE1	13	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	9	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	9	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	9	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	9	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	9	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	9	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	9	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	9	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	9	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	9	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	9	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	9	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	9	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	9	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	9	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	9	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	9	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	9	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	9	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	9	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	9	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	9	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	9	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	9	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	9	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	9	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	9	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	9	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	9	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	9	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	9	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	9	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	9	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	9	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	9	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	17	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	17	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	17	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	17	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	17	0.18
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	17	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	17	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	17	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	17	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	17	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	17	0.18
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	17	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	17	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	17	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	17	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	17	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	17	0.18
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	17	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	17	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	17	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	17	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	17	0.18
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	17	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	17	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	17	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	17	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	17	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	17	0.18
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	17	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	17	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	17	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	17	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	17	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	17	0.18
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	17	0.18
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG11	14	0.18
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG12	14	0.18
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG13	14	0.18
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG21	14	0.18
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG22	14	0.18
(1,437)	1:51:A:LYS:H	1:156:A:VAL:HG23	14	0.18
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	13	0.18
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	13	0.18
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	13	0.18
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	13	0.18
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	13	0.18
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	13	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	10	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	10	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	10	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	10	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	10	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	10	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	10	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	10	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	10	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	10	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	10	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	10	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	10	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	10	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	10	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	10	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	10	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	10	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	10	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	10	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	10	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	10	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	10	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	10	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	10	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	10	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	10	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	10	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	10	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	10	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	10	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	10	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	10	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	10	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	10	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	12	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	12	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	12	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	12	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	12	0.18
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	12	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	12	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	12	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	12	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	12	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	12	0.18
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	12	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	12	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	12	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	12	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	12	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	12	0.18
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	12	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	12	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	12	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	12	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	12	0.18
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	12	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	12	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	12	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	12	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	12	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	12	0.18
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	12	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	12	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	12	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	12	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	12	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	12	0.18
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	12	0.18
(1,403)	1:12:A:LEU:HD11	1:54:A:LEU:HD11	7	0.18
(1,403)	1:12:A:LEU:HD11	1:54:A:LEU:HD12	7	0.18
(1,403)	1:12:A:LEU:HD11	1:54:A:LEU:HD13	7	0.18
(1,403)	1:12:A:LEU:HD11	1:54:A:LEU:HD21	7	0.18
(1,403)	1:12:A:LEU:HD11	1:54:A:LEU:HD22	7	0.18
(1,403)	1:12:A:LEU:HD11	1:54:A:LEU:HD23	7	0.18
(1,403)	1:12:A:LEU:HD12	1:54:A:LEU:HD11	7	0.18
(1,403)	1:12:A:LEU:HD12	1:54:A:LEU:HD12	7	0.18
(1,403)	1:12:A:LEU:HD12	1:54:A:LEU:HD13	7	0.18
(1,403)	1:12:A:LEU:HD12	1:54:A:LEU:HD21	7	0.18
(1,403)	1:12:A:LEU:HD12	1:54:A:LEU:HD22	7	0.18
(1,403)	1:12:A:LEU:HD12	1:54:A:LEU:HD23	7	0.18
(1,403)	1:12:A:LEU:HD13	1:54:A:LEU:HD11	7	0.18
(1,403)	1:12:A:LEU:HD13	1:54:A:LEU:HD12	7	0.18
(1,403)	1:12:A:LEU:HD13	1:54:A:LEU:HD13	7	0.18
(1,403)	1:12:A:LEU:HD13	1:54:A:LEU:HD21	7	0.18
(1,403)	1:12:A:LEU:HD13	1:54:A:LEU:HD22	7	0.18
(1,403)	1:12:A:LEU:HD13	1:54:A:LEU:HD23	7	0.18
(1,403)	1:12:A:LEU:HD21	1:54:A:LEU:HD11	7	0.18
(1,403)	1:12:A:LEU:HD21	1:54:A:LEU:HD12	7	0.18
(1,403)	1:12:A:LEU:HD21	1:54:A:LEU:HD13	7	0.18
(1,403)	1:12:A:LEU:HD21	1:54:A:LEU:HD21	7	0.18
(1,403)	1:12:A:LEU:HD21	1:54:A:LEU:HD22	7	0.18
(1,403)	1:12:A:LEU:HD21	1:54:A:LEU:HD23	7	0.18
(1,403)	1:12:A:LEU:HD22	1:54:A:LEU:HD11	7	0.18
(1,403)	1:12:A:LEU:HD22	1:54:A:LEU:HD12	7	0.18
(1,403)	1:12:A:LEU:HD22	1:54:A:LEU:HD13	7	0.18
(1,403)	1:12:A:LEU:HD22	1:54:A:LEU:HD21	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,403)	1:12:A:LEU:HD22	1:54:A:LEU:HD22	7	0.18
(1,403)	1:12:A:LEU:HD22	1:54:A:LEU:HD23	7	0.18
(1,403)	1:12:A:LEU:HD23	1:54:A:LEU:HD11	7	0.18
(1,403)	1:12:A:LEU:HD23	1:54:A:LEU:HD12	7	0.18
(1,403)	1:12:A:LEU:HD23	1:54:A:LEU:HD13	7	0.18
(1,403)	1:12:A:LEU:HD23	1:54:A:LEU:HD21	7	0.18
(1,403)	1:12:A:LEU:HD23	1:54:A:LEU:HD22	7	0.18
(1,403)	1:12:A:LEU:HD23	1:54:A:LEU:HD23	7	0.18
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	6	0.18
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	6	0.18
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	6	0.18
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD11	9	0.18
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD12	9	0.18
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD13	9	0.18
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD11	9	0.18
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD12	9	0.18
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD13	9	0.18
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD11	9	0.18
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD12	9	0.18
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD13	9	0.18
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	11	0.18
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	11	0.18
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	11	0.18
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	11	0.18
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	11	0.18
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	11	0.18
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	1	0.18
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	1	0.18
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	1	0.18
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	1	0.18
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	1	0.18
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	1	0.18
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	11	0.18
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	11	0.18
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	11	0.18
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	11	0.18
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	11	0.18
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	11	0.18
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	5	0.18
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	13	0.18
(1,263)	1:68:A:ALA:H	1:70:A:SER:H	14	0.18
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:134:A:MET:H	1:136:A:THR:H	17	0.18
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	9	0.18
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	13	0.18
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	20	0.18
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	5	0.18
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	18	0.18
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	5	0.18
(1,212)	1:99:A:VAL:H	1:102:A:GLY:H	15	0.18
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	4	0.18
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	1	0.18
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	11	0.18
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	12	0.18
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	20	0.18
(1,188)	1:119:A:VAL:H	1:121:A:LYS:H	8	0.18
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	4	0.18
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	10	0.18
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	2	0.18
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	4	0.18
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	11	0.18
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	4	0.18
(1,149)	1:129:A:ARG:H	1:131:A:ALA:H	9	0.18
(1,149)	1:129:A:ARG:H	1:131:A:ALA:H	17	0.18
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	6	0.18
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	4	0.18
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	10	0.18
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	11	0.18
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	1	0.18
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	9	0.18
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	10	0.18
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	9	0.18
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	9	0.18
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	13	0.18
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	9	0.18
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	17	0.18
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	9	0.18
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	13	0.18
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	7	0.18
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	4	0.18
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	8	0.18
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	9	0.18
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	15	0.18
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	13	0.18
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	10	0.18
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	4	0.18
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	10	0.18
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	1	0.18
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	10	0.18
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	10	0.18
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	1	0.18
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	2	0.18
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	7	0.18
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	13	0.18
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	8	0.18
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	3	0.18
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	14	0.18
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	10	0.18
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	3	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	3	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	3	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	3	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	3	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	3	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	3	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	3	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	3	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	3	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	3	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	3	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	3	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	3	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	3	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	3	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	3	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	3	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	3	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	3	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	3	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	3	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	3	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	3	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	3	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	3	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	3	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	3	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	3	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	3	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	3	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	3	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	3	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	3	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	3	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	17	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	17	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	17	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	17	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	17	0.17
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	17	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	17	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	17	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	17	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	17	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	17	0.17
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	17	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	17	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	17	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	17	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	17	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	17	0.17
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	17	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	17	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	17	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	17	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	17	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	17	0.17
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	17	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	17	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	17	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	17	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	17	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	17	0.17
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	17	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	17	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	17	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	17	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	17	0.17
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	17	0.17
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	8	0.17
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	8	0.17
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	8	0.17
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	8	0.17
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	8	0.17
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	8	0.17
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	12	0.17
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	12	0.17
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	12	0.17
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	12	0.17
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	12	0.17
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	12	0.17
(1,435)	1:50:A:VAL:HG11	1:153:A:ASP:H	10	0.17
(1,435)	1:50:A:VAL:HG12	1:153:A:ASP:H	10	0.17
(1,435)	1:50:A:VAL:HG13	1:153:A:ASP:H	10	0.17
(1,435)	1:50:A:VAL:HG21	1:153:A:ASP:H	10	0.17
(1,435)	1:50:A:VAL:HG22	1:153:A:ASP:H	10	0.17
(1,435)	1:50:A:VAL:HG23	1:153:A:ASP:H	10	0.17
(1,424)	1:21:A:LEU:HD11	1:118:A:SER:H	6	0.17
(1,424)	1:21:A:LEU:HD12	1:118:A:SER:H	6	0.17
(1,424)	1:21:A:LEU:HD13	1:118:A:SER:H	6	0.17
(1,424)	1:21:A:LEU:HD21	1:118:A:SER:H	6	0.17
(1,424)	1:21:A:LEU:HD22	1:118:A:SER:H	6	0.17
(1,424)	1:21:A:LEU:HD23	1:118:A:SER:H	6	0.17
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	11	0.17
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	11	0.17
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	11	0.17
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	11	0.17
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	11	0.17
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	11	0.17
(1,404)	1:12:A:LEU:HD11	1:152:A:TRP:HE1	16	0.17
(1,404)	1:12:A:LEU:HD12	1:152:A:TRP:HE1	16	0.17
(1,404)	1:12:A:LEU:HD13	1:152:A:TRP:HE1	16	0.17
(1,404)	1:12:A:LEU:HD21	1:152:A:TRP:HE1	16	0.17
(1,404)	1:12:A:LEU:HD22	1:152:A:TRP:HE1	16	0.17
(1,404)	1:12:A:LEU:HD23	1:152:A:TRP:HE1	16	0.17
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD11	2	0.17
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD12	2	0.17
(1,387)	1:104:A:ILE:HD11	1:142:A:LEU:HD13	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD11	2	0.17
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD12	2	0.17
(1,387)	1:104:A:ILE:HD12	1:142:A:LEU:HD13	2	0.17
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD11	2	0.17
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD12	2	0.17
(1,387)	1:104:A:ILE:HD13	1:142:A:LEU:HD13	2	0.17
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	2	0.17
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	2	0.17
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	2	0.17
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	2	0.17
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	2	0.17
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	2	0.17
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	7	0.17
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	7	0.17
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	7	0.17
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	7	0.17
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	7	0.17
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	7	0.17
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD21	3	0.17
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD22	3	0.17
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD23	3	0.17
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD21	3	0.17
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD22	3	0.17
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD23	3	0.17
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD21	3	0.17
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD22	3	0.17
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD23	3	0.17
(1,303)	1:13:A:VAL:HG11	1:134:A:MET:H	18	0.17
(1,303)	1:13:A:VAL:HG12	1:134:A:MET:H	18	0.17
(1,303)	1:13:A:VAL:HG13	1:134:A:MET:H	18	0.17
(1,289)	1:16:A:PHE:H	1:17:A:LEU:HD11	16	0.17
(1,289)	1:16:A:PHE:H	1:17:A:LEU:HD12	16	0.17
(1,289)	1:16:A:PHE:H	1:17:A:LEU:HD13	16	0.17
(1,289)	1:16:A:PHE:H	1:17:A:LEU:HD21	16	0.17
(1,289)	1:16:A:PHE:H	1:17:A:LEU:HD22	16	0.17
(1,289)	1:16:A:PHE:H	1:17:A:LEU:HD23	16	0.17
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	2	0.17
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	3	0.17
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	16	0.17
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	12	0.17
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	19	0.17
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	4	0.17
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	6	0.17
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	14	0.17
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	1	0.17
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	7	0.17
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	19	0.17
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	9	0.17
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	8	0.17
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	15	0.17
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	15	0.17
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	5	0.17
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	15	0.17
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	12	0.17
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	6	0.17
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	16	0.17
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	17	0.17
(1,145)	1:164:A:ALA:H	1:166:A:GLU:H	13	0.17
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	15	0.17
(1,142)	1:95:A:PHE:H	1:97:A:ASP:H	17	0.17
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	3	0.17
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	17	0.17
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	12	0.17
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	1	0.17
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	16	0.17
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	17	0.17
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	9	0.17
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	12	0.17
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	3	0.17
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	20	0.17
(1,105)	1:33:A:ASP:H	1:35:A:GLU:H	4	0.17
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	11	0.17
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	3	0.17
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	7	0.17
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	10	0.17
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	12	0.17
(1,90)	1:8:A:SER:H	1:10:A:ARG:H	3	0.17
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	14	0.17
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	1	0.17
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	1	0.17
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	8	0.17
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	16	0.17
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	10	0.17
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	3	0.17
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	1	0.17
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	4	0.17
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	14	0.17
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	3	0.17
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	7	0.17
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	9	0.17
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	2	0.17
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	15	0.17
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	13	0.17
(1,34)	1:141:A:HIS:H	1:143:A:GLU:H	16	0.17
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	18	0.17
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	8	0.17
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	18	0.17
(1,17)	1:106:A:ALA:H	1:109:A:SER:H	1	0.17
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	6	0.17
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	15	0.17
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	9	0.17
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	18	0.17
(1,505)	1:138:A:LEU:HD11	1:152:A:TRP:HE1	8	0.16
(1,505)	1:138:A:LEU:HD12	1:152:A:TRP:HE1	8	0.16
(1,505)	1:138:A:LEU:HD13	1:152:A:TRP:HE1	8	0.16
(1,505)	1:138:A:LEU:HD21	1:152:A:TRP:HE1	8	0.16
(1,505)	1:138:A:LEU:HD22	1:152:A:TRP:HE1	8	0.16
(1,505)	1:138:A:LEU:HD23	1:152:A:TRP:HE1	8	0.16
(1,481)	1:104:A:ILE:HD11	1:142:A:LEU:HD11	20	0.16
(1,481)	1:104:A:ILE:HD11	1:142:A:LEU:HD12	20	0.16
(1,481)	1:104:A:ILE:HD11	1:142:A:LEU:HD13	20	0.16
(1,481)	1:104:A:ILE:HD11	1:142:A:LEU:HD21	20	0.16
(1,481)	1:104:A:ILE:HD11	1:142:A:LEU:HD22	20	0.16
(1,481)	1:104:A:ILE:HD11	1:142:A:LEU:HD23	20	0.16
(1,481)	1:104:A:ILE:HD12	1:142:A:LEU:HD11	20	0.16
(1,481)	1:104:A:ILE:HD12	1:142:A:LEU:HD12	20	0.16
(1,481)	1:104:A:ILE:HD12	1:142:A:LEU:HD13	20	0.16
(1,481)	1:104:A:ILE:HD12	1:142:A:LEU:HD21	20	0.16
(1,481)	1:104:A:ILE:HD12	1:142:A:LEU:HD22	20	0.16
(1,481)	1:104:A:ILE:HD12	1:142:A:LEU:HD23	20	0.16
(1,481)	1:104:A:ILE:HD13	1:142:A:LEU:HD11	20	0.16
(1,481)	1:104:A:ILE:HD13	1:142:A:LEU:HD12	20	0.16
(1,481)	1:104:A:ILE:HD13	1:142:A:LEU:HD13	20	0.16
(1,481)	1:104:A:ILE:HD13	1:142:A:LEU:HD21	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:104:A:ILE:HD13	1:142:A:LEU:HD22	20	0.16
(1,481)	1:104:A:ILE:HD13	1:142:A:LEU:HD23	20	0.16
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	11	0.16
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	11	0.16
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	11	0.16
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	11	0.16
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	11	0.16
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	11	0.16
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	12	0.16
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	12	0.16
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	12	0.16
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	12	0.16
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	12	0.16
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	12	0.16
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	2	0.16
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	2	0.16
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	2	0.16
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	2	0.16
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	2	0.16
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	2	0.16
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	4	0.16
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	4	0.16
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	4	0.16
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	4	0.16
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	4	0.16
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	4	0.16
(1,454)	1:72:A:LEU:HD11	1:111:A:GLY:H	1	0.16
(1,454)	1:72:A:LEU:HD12	1:111:A:GLY:H	1	0.16
(1,454)	1:72:A:LEU:HD13	1:111:A:GLY:H	1	0.16
(1,454)	1:72:A:LEU:HD21	1:111:A:GLY:H	1	0.16
(1,454)	1:72:A:LEU:HD22	1:111:A:GLY:H	1	0.16
(1,454)	1:72:A:LEU:HD23	1:111:A:GLY:H	1	0.16
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG11	14	0.16
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG12	14	0.16
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG13	14	0.16
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG21	14	0.16
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG22	14	0.16
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG23	14	0.16
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG11	14	0.16
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG12	14	0.16
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG13	14	0.16
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG21	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG22	14	0.16
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG23	14	0.16
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG11	14	0.16
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG12	14	0.16
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG13	14	0.16
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG21	14	0.16
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG22	14	0.16
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG23	14	0.16
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG11	14	0.16
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG12	14	0.16
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG13	14	0.16
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG21	14	0.16
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG22	14	0.16
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG23	14	0.16
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG11	14	0.16
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG12	14	0.16
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG13	14	0.16
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG21	14	0.16
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG22	14	0.16
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG23	14	0.16
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG11	14	0.16
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG12	14	0.16
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG13	14	0.16
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG21	14	0.16
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG22	14	0.16
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG23	14	0.16
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD21	16	0.16
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD22	16	0.16
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD23	16	0.16
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD21	16	0.16
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD22	16	0.16
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD23	16	0.16
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD21	16	0.16
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD22	16	0.16
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD23	16	0.16
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG11	14	0.16
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG12	14	0.16
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG13	14	0.16
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG21	14	0.16
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG22	14	0.16
(1,321)	1:21:A:LEU:H	1:116:A:VAL:HG23	14	0.16
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	5	0.16
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	6	0.16
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	19	0.16
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	20	0.16
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	4	0.16
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	7	0.16
(1,244)	1:22:A:SER:H	1:24:A:LYS:H	1	0.16
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	5	0.16
(1,232)	1:67:A:ARG:H	1:68:A:ALA:H	8	0.16
(1,231)	1:66:A:ARG:H	1:67:A:ARG:H	18	0.16
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	17	0.16
(1,218)	1:13:A:VAL:H	1:15:A:ASP:H	20	0.16
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	19	0.16
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	3	0.16
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	6	0.16
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	17	0.16
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	2	0.16
(1,158)	1:102:A:GLY:H	1:104:A:ILE:H	9	0.16
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	18	0.16
(1,152)	1:127:A:VAL:H	1:129:A:ARG:H	3	0.16
(1,152)	1:127:A:VAL:H	1:129:A:ARG:H	5	0.16
(1,152)	1:127:A:VAL:H	1:129:A:ARG:H	12	0.16
(1,149)	1:129:A:ARG:H	1:131:A:ALA:H	4	0.16
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	17	0.16
(1,133)	1:117:A:GLU:H	1:119:A:VAL:H	14	0.16
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	5	0.16
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	2	0.16
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	11	0.16
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	19	0.16
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	1	0.16
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	4	0.16
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	14	0.16
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	16	0.16
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	4	0.16
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	8	0.16
(1,91)	1:10:A:ARG:H	1:12:A:LEU:H	1	0.16
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	19	0.16
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	8	0.16
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	18	0.16
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	16	0.16
(1,72)	1:88:A:GLU:H	1:91:A:VAL:H	13	0.16
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	9	0.16
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	1	0.16
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	10	0.16
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	9	0.16
(1,8)	1:44:A:GLY:H	1:45:A:THR:H	17	0.16
(1,7)	1:91:A:VAL:H	1:93:A:GLU:H	17	0.16
(1,5)	1:65:A:TYR:H	1:66:A:ARG:H	13	0.16
(2,7)	1:104:A:ILE:HD11	1:145:A:TRP:H	8	0.15
(2,7)	1:104:A:ILE:HD12	1:145:A:TRP:H	8	0.15
(2,7)	1:104:A:ILE:HD13	1:145:A:TRP:H	8	0.15
(2,6)	1:78:A:ILE:HD11	1:128:A:SER:H	7	0.15
(2,6)	1:78:A:ILE:HD12	1:128:A:SER:H	7	0.15
(2,6)	1:78:A:ILE:HD13	1:128:A:SER:H	7	0.15
(2,4)	1:10:A:ARG:H	1:152:A:TRP:HE1	4	0.15
(1,505)	1:138:A:LEU:HD11	1:152:A:TRP:HE1	20	0.15
(1,505)	1:138:A:LEU:HD12	1:152:A:TRP:HE1	20	0.15
(1,505)	1:138:A:LEU:HD13	1:152:A:TRP:HE1	20	0.15
(1,505)	1:138:A:LEU:HD21	1:152:A:TRP:HE1	20	0.15
(1,505)	1:138:A:LEU:HD22	1:152:A:TRP:HE1	20	0.15
(1,505)	1:138:A:LEU:HD23	1:152:A:TRP:HE1	20	0.15
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	1	0.15
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	1	0.15
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	1	0.15
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	1	0.15
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	1	0.15
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	1	0.15
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	1	0.15
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	1	0.15
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	1	0.15
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	1	0.15
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	1	0.15
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	1	0.15
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	1	0.15
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	1	0.15
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	1	0.15
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	1	0.15
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	1	0.15
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	1	0.15
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	1	0.15
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	1	0.15
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	1	0.15
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	1	0.15
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	1	0.15
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	1	0.15
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	1	0.15
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	1	0.15
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	1	0.15
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	1	0.15
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	1	0.15
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	1	0.15
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	1	0.15
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	1	0.15
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	1	0.15
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	1	0.15
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	1	0.15
(1,434)	1:50:A:VAL:HG11	1:152:A:TRP:H	15	0.15
(1,434)	1:50:A:VAL:HG12	1:152:A:TRP:H	15	0.15
(1,434)	1:50:A:VAL:HG13	1:152:A:TRP:H	15	0.15
(1,434)	1:50:A:VAL:HG21	1:152:A:TRP:H	15	0.15
(1,434)	1:50:A:VAL:HG22	1:152:A:TRP:H	15	0.15
(1,434)	1:50:A:VAL:HG23	1:152:A:TRP:H	15	0.15
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG11	2	0.15
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG12	2	0.15
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG13	2	0.15
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG21	2	0.15
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG22	2	0.15
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG23	2	0.15
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG11	2	0.15
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG12	2	0.15
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG13	2	0.15
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG21	2	0.15
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG22	2	0.15
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG23	2	0.15
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG11	2	0.15
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG12	2	0.15
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG13	2	0.15
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG21	2	0.15
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG22	2	0.15
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG23	2	0.15
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG11	2	0.15
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG12	2	0.15
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG13	2	0.15
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG21	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG22	2	0.15
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG23	2	0.15
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG11	2	0.15
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG12	2	0.15
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG13	2	0.15
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG21	2	0.15
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG22	2	0.15
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG23	2	0.15
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG11	2	0.15
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG12	2	0.15
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG13	2	0.15
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG21	2	0.15
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG22	2	0.15
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG23	2	0.15
(1,404)	1:12:A:LEU:HD11	1:152:A:TRP:HE1	7	0.15
(1,404)	1:12:A:LEU:HD12	1:152:A:TRP:HE1	7	0.15
(1,404)	1:12:A:LEU:HD13	1:152:A:TRP:HE1	7	0.15
(1,404)	1:12:A:LEU:HD21	1:152:A:TRP:HE1	7	0.15
(1,404)	1:12:A:LEU:HD22	1:152:A:TRP:HE1	7	0.15
(1,404)	1:12:A:LEU:HD23	1:152:A:TRP:HE1	7	0.15
(1,394)	1:138:A:LEU:HD11	1:143:A:GLU:H	15	0.15
(1,394)	1:138:A:LEU:HD12	1:143:A:GLU:H	15	0.15
(1,394)	1:138:A:LEU:HD13	1:143:A:GLU:H	15	0.15
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD11	18	0.15
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD12	18	0.15
(1,326)	1:114:A:LEU:H	1:130:A:ILE:HD13	18	0.15
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	9	0.15
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	1	0.15
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	17	0.15
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	18	0.15
(1,234)	1:116:A:VAL:H	1:117:A:GLU:H	6	0.15
(1,231)	1:66:A:ARG:H	1:67:A:ARG:H	13	0.15
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	8	0.15
(1,223)	1:52:A:GLN:H	1:56:A:GLU:H	17	0.15
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	1	0.15
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	6	0.15
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	7	0.15
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	1	0.15
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	16	0.15
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	2	0.15
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	13	0.15
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:55:A:ARG:H	1:57:A:ALA:H	16	0.15
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	9	0.15
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	14	0.15
(1,189)	1:69:A:PHE:H	1:72:A:LEU:H	7	0.15
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	11	0.15
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	8	0.15
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	20	0.15
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	3	0.15
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	10	0.15
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	12	0.15
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	5	0.15
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	9	0.15
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	13	0.15
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	1	0.15
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	6	0.15
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	5	0.15
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	7	0.15
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	19	0.15
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	9	0.15
(1,112)	1:28:A:TRP:H	1:30:A:GLN:H	7	0.15
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	15	0.15
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	17	0.15
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	2	0.15
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	6	0.15
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	19	0.15
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	12	0.15
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	20	0.15
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	20	0.15
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	1	0.15
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	11	0.15
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	16	0.15
(1,80)	1:126:A:LEU:H	1:128:A:SER:H	9	0.15
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	13	0.15
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	19	0.15
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	8	0.15
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	17	0.15
(1,68)	1:158:A:LEU:H	1:161:A:ASN:H	5	0.15
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	3	0.15
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	6	0.15
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	15	0.15
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	20	0.15
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	12	0.15
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	20	0.15
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	11	0.15
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	12	0.15
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	15	0.15
(1,20)	1:44:A:GLY:H	1:46:A:GLU:H	7	0.15
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	17	0.15
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	18	0.15
(1,14)	1:92:A:ASN:H	1:94:A:LEU:H	11	0.15
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	5	0.15
(1,3)	1:72:A:LEU:H	1:74:A:SER:H	7	0.15
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD11	5	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD12	5	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD13	5	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD21	5	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD22	5	0.14
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD23	5	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG11	20	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG12	20	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG13	20	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG21	20	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG22	20	0.14
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG23	20	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG11	20	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG12	20	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG13	20	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG21	20	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG22	20	0.14
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG23	20	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG11	20	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG12	20	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG13	20	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG21	20	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG22	20	0.14
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG23	20	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG11	20	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG12	20	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG13	20	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG21	20	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG22	20	0.14
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG23	20	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG11	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG12	20	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG13	20	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG21	20	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG22	20	0.14
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG23	20	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG11	20	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG12	20	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG13	20	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG21	20	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG22	20	0.14
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG23	20	0.14
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD11	6	0.14
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD12	6	0.14
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD13	6	0.14
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD21	6	0.14
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD22	6	0.14
(1,463)	1:91:A:VAL:HG11	1:94:A:LEU:HD23	6	0.14
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD11	6	0.14
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD12	6	0.14
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD13	6	0.14
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD21	6	0.14
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD22	6	0.14
(1,463)	1:91:A:VAL:HG12	1:94:A:LEU:HD23	6	0.14
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD11	6	0.14
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD12	6	0.14
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD13	6	0.14
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD21	6	0.14
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD22	6	0.14
(1,463)	1:91:A:VAL:HG13	1:94:A:LEU:HD23	6	0.14
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD11	6	0.14
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD12	6	0.14
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD13	6	0.14
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD21	6	0.14
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD22	6	0.14
(1,463)	1:91:A:VAL:HG21	1:94:A:LEU:HD23	6	0.14
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD11	6	0.14
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD12	6	0.14
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD13	6	0.14
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD21	6	0.14
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD22	6	0.14
(1,463)	1:91:A:VAL:HG22	1:94:A:LEU:HD23	6	0.14
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD11	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD12	6	0.14
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD13	6	0.14
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD21	6	0.14
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD22	6	0.14
(1,463)	1:91:A:VAL:HG23	1:94:A:LEU:HD23	6	0.14
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	10	0.14
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	10	0.14
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	10	0.14
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	10	0.14
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	10	0.14
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	10	0.14
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	4	0.14
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	4	0.14
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	4	0.14
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	4	0.14
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	4	0.14
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	4	0.14
(1,448)	1:72:A:LEU:HD11	1:90:A:VAL:H	14	0.14
(1,448)	1:72:A:LEU:HD12	1:90:A:VAL:H	14	0.14
(1,448)	1:72:A:LEU:HD13	1:90:A:VAL:H	14	0.14
(1,448)	1:72:A:LEU:HD21	1:90:A:VAL:H	14	0.14
(1,448)	1:72:A:LEU:HD22	1:90:A:VAL:H	14	0.14
(1,448)	1:72:A:LEU:HD23	1:90:A:VAL:H	14	0.14
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	7	0.14
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	7	0.14
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	7	0.14
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	7	0.14
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	7	0.14
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	7	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	2	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	2	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	2	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	2	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	2	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	2	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD11	15	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD12	15	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD13	15	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD21	15	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD22	15	0.14
(1,417)	1:15:A:ASP:H	1:54:A:LEU:HD23	15	0.14
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	19	0.14
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	19	0.14
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	8	0.14
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	8	0.14
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	8	0.14
(1,394)	1:138:A:LEU:HD11	1:143:A:GLU:H	4	0.14
(1,394)	1:138:A:LEU:HD12	1:143:A:GLU:H	4	0.14
(1,394)	1:138:A:LEU:HD13	1:143:A:GLU:H	4	0.14
(1,338)	1:12:A:LEU:HD21	1:51:A:LYS:H	10	0.14
(1,338)	1:12:A:LEU:HD22	1:51:A:LYS:H	10	0.14
(1,338)	1:12:A:LEU:HD23	1:51:A:LYS:H	10	0.14
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	1	0.14
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	1	0.14
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	1	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	1	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	4	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	6	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	8	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	10	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	12	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	15	0.14
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	18	0.14
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	16	0.14
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	17	0.14
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	13	0.14
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	15	0.14
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	5	0.14
(1,246)	1:22:A:SER:H	1:26:A:TYR:H	2	0.14
(1,230)	1:21:A:LEU:H	1:23:A:GLN:H	14	0.14
(1,217)	1:23:A:GLN:H	1:26:A:TYR:H	17	0.14
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	16	0.14
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	19	0.14
(1,212)	1:99:A:VAL:H	1:102:A:GLY:H	8	0.14
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	9	0.14
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	20	0.14
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	2	0.14
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	3	0.14
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	20	0.14
(1,203)	1:116:A:VAL:H	1:118:A:SER:H	9	0.14
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	18	0.14
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	7	0.14
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	2	0.14
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	2	0.14
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	3	0.14
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	16	0.14
(1,177)	1:156:A:VAL:H	1:159:A:TYR:H	8	0.14
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	1	0.14
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	8	0.14
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	14	0.14
(1,173)	1:118:A:SER:H	1:120:A:ASP:H	10	0.14
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	7	0.14
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	19	0.14
(1,157)	1:104:A:ILE:H	1:106:A:ALA:H	3	0.14
(1,152)	1:127:A:VAL:H	1:129:A:ARG:H	13	0.14
(1,145)	1:164:A:ALA:H	1:166:A:GLU:H	7	0.14
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	17	0.14
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	18	0.14
(1,119)	1:56:A:GLU:H	1:58:A:GLY:H	12	0.14
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	6	0.14
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	18	0.14
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	17	0.14
(1,113)	1:22:A:SER:H	1:25:A:GLY:H	18	0.14
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	1	0.14
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	10	0.14
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	16	0.14
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	10	0.14
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	17	0.14
(1,105)	1:33:A:ASP:H	1:35:A:GLU:H	15	0.14
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	12	0.14
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	4	0.14
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	9	0.14
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	15	0.14
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	7	0.14
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	8	0.14
(1,79)	1:27:A:SER:H	1:30:A:GLN:H	17	0.14
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	18	0.14
(1,69)	1:156:A:VAL:H	1:158:A:LEU:H	19	0.14
(1,68)	1:158:A:LEU:H	1:161:A:ASN:H	8	0.14
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	12	0.14
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	5	0.14
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	6	0.14
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	19	0.14
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:59:A:ASP:H	1:61:A:PHE:H	5	0.14
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	6	0.14
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	18	0.14
(1,35)	1:131:A:ALA:H	1:133:A:TRP:H	9	0.14
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	4	0.14
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	16	0.14
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	4	0.14
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	11	0.14
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	13	0.14
(1,5)	1:65:A:TYR:H	1:66:A:ARG:H	18	0.14
(1,511)	1:158:A:LEU:HD11	1:160:A:GLY:H	6	0.13
(1,511)	1:158:A:LEU:HD12	1:160:A:GLY:H	6	0.13
(1,511)	1:158:A:LEU:HD13	1:160:A:GLY:H	6	0.13
(1,511)	1:158:A:LEU:HD21	1:160:A:GLY:H	6	0.13
(1,511)	1:158:A:LEU:HD22	1:160:A:GLY:H	6	0.13
(1,511)	1:158:A:LEU:HD23	1:160:A:GLY:H	6	0.13
(1,511)	1:158:A:LEU:HD11	1:160:A:GLY:H	8	0.13
(1,511)	1:158:A:LEU:HD12	1:160:A:GLY:H	8	0.13
(1,511)	1:158:A:LEU:HD13	1:160:A:GLY:H	8	0.13
(1,511)	1:158:A:LEU:HD21	1:160:A:GLY:H	8	0.13
(1,511)	1:158:A:LEU:HD22	1:160:A:GLY:H	8	0.13
(1,511)	1:158:A:LEU:HD23	1:160:A:GLY:H	8	0.13
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	2	0.13
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	2	0.13
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	2	0.13
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	2	0.13
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	2	0.13
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	2	0.13
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	2	0.13
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	2	0.13
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	2	0.13
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	2	0.13
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	2	0.13
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	2	0.13
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	2	0.13
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	2	0.13
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	2	0.13
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	2	0.13
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	2	0.13
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	2	0.13
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	2	0.13
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	2	0.13
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	2	0.13
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	2	0.13
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	2	0.13
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	2	0.13
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	2	0.13
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	2	0.13
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	2	0.13
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	2	0.13
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	2	0.13
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	2	0.13
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	2	0.13
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	2	0.13
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	2	0.13
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	2	0.13
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	2	0.13
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	6	0.13
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	6	0.13
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	6	0.13
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	6	0.13
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	6	0.13
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	6	0.13
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	18	0.13
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	18	0.13
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	18	0.13
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	18	0.13
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	18	0.13
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	18	0.13
(1,423)	1:21:A:LEU:HD11	1:28:A:TRP:HE1	8	0.13
(1,423)	1:21:A:LEU:HD12	1:28:A:TRP:HE1	8	0.13
(1,423)	1:21:A:LEU:HD13	1:28:A:TRP:HE1	8	0.13
(1,423)	1:21:A:LEU:HD21	1:28:A:TRP:HE1	8	0.13
(1,423)	1:21:A:LEU:HD22	1:28:A:TRP:HE1	8	0.13
(1,423)	1:21:A:LEU:HD23	1:28:A:TRP:HE1	8	0.13
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	13	0.13
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	13	0.13
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	13	0.13
(1,397)	1:138:A:LEU:HD11	1:142:A:LEU:H	2	0.13
(1,397)	1:138:A:LEU:HD12	1:142:A:LEU:H	2	0.13
(1,397)	1:138:A:LEU:HD13	1:142:A:LEU:H	2	0.13
(1,377)	1:17:A:LEU:HD11	1:111:A:GLY:H	8	0.13
(1,377)	1:17:A:LEU:HD12	1:111:A:GLY:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:17:A:LEU:HD13	1:111:A:GLY:H	8	0.13
(1,377)	1:17:A:LEU:HD21	1:111:A:GLY:H	8	0.13
(1,377)	1:17:A:LEU:HD22	1:111:A:GLY:H	8	0.13
(1,377)	1:17:A:LEU:HD23	1:111:A:GLY:H	8	0.13
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD21	20	0.13
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD22	20	0.13
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD23	20	0.13
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD21	20	0.13
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD22	20	0.13
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD23	20	0.13
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD21	20	0.13
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD22	20	0.13
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD23	20	0.13
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	7	0.13
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	7	0.13
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	7	0.13
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	7	0.13
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	7	0.13
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	7	0.13
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	11	0.13
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	8	0.13
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	17	0.13
(1,263)	1:68:A:ALA:H	1:70:A:SER:H	12	0.13
(1,258)	1:47:A:SER:H	1:49:A:ALA:H	10	0.13
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	7	0.13
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	11	0.13
(1,234)	1:116:A:VAL:H	1:117:A:GLU:H	19	0.13
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	18	0.13
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	16	0.13
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	18	0.13
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	7	0.13
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	8	0.13
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	11	0.13
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	14	0.13
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	5	0.13
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	18	0.13
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	8	0.13
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	2	0.13
(1,177)	1:156:A:VAL:H	1:159:A:TYR:H	17	0.13
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	18	0.13
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	18	0.13
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	5	0.13
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	6	0.13
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	15	0.13
(1,150)	1:126:A:LEU:H	1:129:A:ARG:H	14	0.13
(1,145)	1:164:A:ALA:H	1:166:A:GLU:H	19	0.13
(1,143)	1:132:A:ALA:H	1:134:A:MET:H	2	0.13
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	19	0.13
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	8	0.13
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	13	0.13
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	20	0.13
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	9	0.13
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	11	0.13
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	14	0.13
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	2	0.13
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	4	0.13
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	7	0.13
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	11	0.13
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	18	0.13
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	20	0.13
(1,91)	1:10:A:ARG:H	1:12:A:LEU:H	15	0.13
(1,90)	1:8:A:SER:H	1:10:A:ARG:H	13	0.13
(1,90)	1:8:A:SER:H	1:10:A:ARG:H	19	0.13
(1,86)	1:19:A:TYR:H	1:21:A:LEU:H	8	0.13
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	4	0.13
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	3	0.13
(1,79)	1:27:A:SER:H	1:30:A:GLN:H	19	0.13
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	5	0.13
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	15	0.13
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	12	0.13
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	11	0.13
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	17	0.13
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	4	0.13
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	5	0.13
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	9	0.13
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	20	0.13
(1,17)	1:106:A:ALA:H	1:109:A:SER:H	17	0.13
(1,14)	1:92:A:ASN:H	1:94:A:LEU:H	10	0.13
(1,14)	1:92:A:ASN:H	1:94:A:LEU:H	14	0.13
(1,14)	1:92:A:ASN:H	1:94:A:LEU:H	17	0.13
(1,5)	1:65:A:TYR:H	1:66:A:ARG:H	8	0.13
(1,505)	1:138:A:LEU:HD11	1:152:A:TRP:HE1	11	0.12
(1,505)	1:138:A:LEU:HD12	1:152:A:TRP:HE1	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,505)	1:138:A:LEU:HD13	1:152:A:TRP:HE1	11	0.12
(1,505)	1:138:A:LEU:HD21	1:152:A:TRP:HE1	11	0.12
(1,505)	1:138:A:LEU:HD22	1:152:A:TRP:HE1	11	0.12
(1,505)	1:138:A:LEU:HD23	1:152:A:TRP:HE1	11	0.12
(1,504)	1:138:A:LEU:HD11	1:142:A:LEU:HD11	8	0.12
(1,504)	1:138:A:LEU:HD11	1:142:A:LEU:HD12	8	0.12
(1,504)	1:138:A:LEU:HD11	1:142:A:LEU:HD13	8	0.12
(1,504)	1:138:A:LEU:HD11	1:142:A:LEU:HD21	8	0.12
(1,504)	1:138:A:LEU:HD11	1:142:A:LEU:HD22	8	0.12
(1,504)	1:138:A:LEU:HD11	1:142:A:LEU:HD23	8	0.12
(1,504)	1:138:A:LEU:HD12	1:142:A:LEU:HD11	8	0.12
(1,504)	1:138:A:LEU:HD12	1:142:A:LEU:HD12	8	0.12
(1,504)	1:138:A:LEU:HD12	1:142:A:LEU:HD13	8	0.12
(1,504)	1:138:A:LEU:HD12	1:142:A:LEU:HD21	8	0.12
(1,504)	1:138:A:LEU:HD12	1:142:A:LEU:HD22	8	0.12
(1,504)	1:138:A:LEU:HD12	1:142:A:LEU:HD23	8	0.12
(1,504)	1:138:A:LEU:HD13	1:142:A:LEU:HD11	8	0.12
(1,504)	1:138:A:LEU:HD13	1:142:A:LEU:HD12	8	0.12
(1,504)	1:138:A:LEU:HD13	1:142:A:LEU:HD13	8	0.12
(1,504)	1:138:A:LEU:HD13	1:142:A:LEU:HD21	8	0.12
(1,504)	1:138:A:LEU:HD13	1:142:A:LEU:HD22	8	0.12
(1,504)	1:138:A:LEU:HD13	1:142:A:LEU:HD23	8	0.12
(1,504)	1:138:A:LEU:HD21	1:142:A:LEU:HD11	8	0.12
(1,504)	1:138:A:LEU:HD21	1:142:A:LEU:HD12	8	0.12
(1,504)	1:138:A:LEU:HD21	1:142:A:LEU:HD13	8	0.12
(1,504)	1:138:A:LEU:HD21	1:142:A:LEU:HD21	8	0.12
(1,504)	1:138:A:LEU:HD21	1:142:A:LEU:HD22	8	0.12
(1,504)	1:138:A:LEU:HD21	1:142:A:LEU:HD23	8	0.12
(1,504)	1:138:A:LEU:HD22	1:142:A:LEU:HD11	8	0.12
(1,504)	1:138:A:LEU:HD22	1:142:A:LEU:HD12	8	0.12
(1,504)	1:138:A:LEU:HD22	1:142:A:LEU:HD13	8	0.12
(1,504)	1:138:A:LEU:HD22	1:142:A:LEU:HD21	8	0.12
(1,504)	1:138:A:LEU:HD22	1:142:A:LEU:HD22	8	0.12
(1,504)	1:138:A:LEU:HD22	1:142:A:LEU:HD23	8	0.12
(1,504)	1:138:A:LEU:HD23	1:142:A:LEU:HD11	8	0.12
(1,504)	1:138:A:LEU:HD23	1:142:A:LEU:HD12	8	0.12
(1,504)	1:138:A:LEU:HD23	1:142:A:LEU:HD13	8	0.12
(1,504)	1:138:A:LEU:HD23	1:142:A:LEU:HD21	8	0.12
(1,504)	1:138:A:LEU:HD23	1:142:A:LEU:HD22	8	0.12
(1,504)	1:138:A:LEU:HD23	1:142:A:LEU:HD23	8	0.12
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD11	8	0.12
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD13	8	0.12
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD21	8	0.12
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD22	8	0.12
(1,477)	1:100:A:ASN:H	1:142:A:LEU:HD23	8	0.12
(1,466)	1:94:A:LEU:HD11	1:106:A:ALA:H	11	0.12
(1,466)	1:94:A:LEU:HD12	1:106:A:ALA:H	11	0.12
(1,466)	1:94:A:LEU:HD13	1:106:A:ALA:H	11	0.12
(1,466)	1:94:A:LEU:HD21	1:106:A:ALA:H	11	0.12
(1,466)	1:94:A:LEU:HD22	1:106:A:ALA:H	11	0.12
(1,466)	1:94:A:LEU:HD23	1:106:A:ALA:H	11	0.12
(1,450)	1:72:A:LEU:HD11	1:93:A:GLU:H	19	0.12
(1,450)	1:72:A:LEU:HD12	1:93:A:GLU:H	19	0.12
(1,450)	1:72:A:LEU:HD13	1:93:A:GLU:H	19	0.12
(1,450)	1:72:A:LEU:HD21	1:93:A:GLU:H	19	0.12
(1,450)	1:72:A:LEU:HD22	1:93:A:GLU:H	19	0.12
(1,450)	1:72:A:LEU:HD23	1:93:A:GLU:H	19	0.12
(1,399)	1:72:A:LEU:HD11	1:110:A:PHE:H	2	0.12
(1,399)	1:72:A:LEU:HD12	1:110:A:PHE:H	2	0.12
(1,399)	1:72:A:LEU:HD13	1:110:A:PHE:H	2	0.12
(1,366)	1:78:A:ILE:HD11	1:130:A:ILE:HD11	3	0.12
(1,366)	1:78:A:ILE:HD11	1:130:A:ILE:HD12	3	0.12
(1,366)	1:78:A:ILE:HD11	1:130:A:ILE:HD13	3	0.12
(1,366)	1:78:A:ILE:HD12	1:130:A:ILE:HD11	3	0.12
(1,366)	1:78:A:ILE:HD12	1:130:A:ILE:HD12	3	0.12
(1,366)	1:78:A:ILE:HD12	1:130:A:ILE:HD13	3	0.12
(1,366)	1:78:A:ILE:HD13	1:130:A:ILE:HD11	3	0.12
(1,366)	1:78:A:ILE:HD13	1:130:A:ILE:HD12	3	0.12
(1,366)	1:78:A:ILE:HD13	1:130:A:ILE:HD13	3	0.12
(1,363)	1:99:A:VAL:HG21	1:101:A:TRP:HE1	11	0.12
(1,363)	1:99:A:VAL:HG22	1:101:A:TRP:HE1	11	0.12
(1,363)	1:99:A:VAL:HG23	1:101:A:TRP:HE1	11	0.12
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	17	0.12
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	17	0.12
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	17	0.12
(1,294)	1:100:A:ASN:H	1:104:A:ILE:HD11	8	0.12
(1,294)	1:100:A:ASN:H	1:104:A:ILE:HD12	8	0.12
(1,294)	1:100:A:ASN:H	1:104:A:ILE:HD13	8	0.12
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	7	0.12
(1,268)	1:162:A:ASN:H	1:163:A:ALA:H	3	0.12
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	1	0.12
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	10	0.12
(1,267)	1:58:A:GLY:H	1:60:A:GLU:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:113:A:ALA:H	1:114:A:LEU:H	17	0.12
(1,263)	1:68:A:ALA:H	1:70:A:SER:H	4	0.12
(1,255)	1:149:A:ASN:H	1:151:A:GLY:H	8	0.12
(1,235)	1:158:A:LEU:H	1:160:A:GLY:H	12	0.12
(1,234)	1:116:A:VAL:H	1:117:A:GLU:H	20	0.12
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	10	0.12
(1,208)	1:108:A:PHE:H	1:110:A:PHE:H	1	0.12
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	9	0.12
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	12	0.12
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	3	0.12
(1,199)	1:90:A:VAL:H	1:92:A:ASN:H	8	0.12
(1,191)	1:101:A:TRP:H	1:102:A:GLY:H	15	0.12
(1,189)	1:69:A:PHE:H	1:72:A:LEU:H	18	0.12
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	1	0.12
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	10	0.12
(1,177)	1:156:A:VAL:H	1:159:A:TYR:H	18	0.12
(1,170)	1:40:A:GLU:H	1:41:A:ALA:H	8	0.12
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	17	0.12
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	18	0.12
(1,158)	1:102:A:GLY:H	1:104:A:ILE:H	17	0.12
(1,149)	1:129:A:ARG:H	1:131:A:ALA:H	8	0.12
(1,145)	1:164:A:ALA:H	1:166:A:GLU:H	1	0.12
(1,145)	1:164:A:ALA:H	1:166:A:GLU:H	2	0.12
(1,145)	1:164:A:ALA:H	1:166:A:GLU:H	14	0.12
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	14	0.12
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	19	0.12
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	15	0.12
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	12	0.12
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	18	0.12
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	2	0.12
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	6	0.12
(1,110)	1:61:A:PHE:H	1:63:A:LEU:H	7	0.12
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	7	0.12
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	11	0.12
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	13	0.12
(1,106)	1:145:A:TRP:H	1:147:A:GLN:H	15	0.12
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	5	0.12
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	11	0.12
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	19	0.12
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	7	0.12
(1,91)	1:10:A:ARG:H	1:12:A:LEU:H	3	0.12
(1,90)	1:8:A:SER:H	1:10:A:ARG:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:124:A:GLN:H	1:126:A:LEU:H	5	0.12
(1,68)	1:158:A:LEU:H	1:161:A:ASN:H	4	0.12
(1,68)	1:158:A:LEU:H	1:161:A:ASN:H	19	0.12
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	18	0.12
(1,61)	1:16:A:PHE:H	1:18:A:SER:H	19	0.12
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	5	0.12
(1,35)	1:131:A:ALA:H	1:133:A:TRP:H	2	0.12
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	3	0.12
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	17	0.12
(1,24)	1:103:A:ARG:H	1:105:A:VAL:H	19	0.12
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	5	0.12
(1,18)	1:32:A:SER:H	1:33:A:ASP:H	14	0.12
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	14	0.12
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	16	0.12
(1,491)	1:125:A:VAL:HG11	1:126:A:LEU:H	12	0.11
(1,491)	1:125:A:VAL:HG12	1:126:A:LEU:H	12	0.11
(1,491)	1:125:A:VAL:HG13	1:126:A:LEU:H	12	0.11
(1,491)	1:125:A:VAL:HG21	1:126:A:LEU:H	12	0.11
(1,491)	1:125:A:VAL:HG22	1:126:A:LEU:H	12	0.11
(1,491)	1:125:A:VAL:HG23	1:126:A:LEU:H	12	0.11
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD11	20	0.11
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD12	20	0.11
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD13	20	0.11
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD21	20	0.11
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD22	20	0.11
(1,474)	1:99:A:VAL:HG11	1:142:A:LEU:HD23	20	0.11
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD11	20	0.11
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD12	20	0.11
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD13	20	0.11
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD21	20	0.11
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD22	20	0.11
(1,474)	1:99:A:VAL:HG12	1:142:A:LEU:HD23	20	0.11
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD11	20	0.11
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD12	20	0.11
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD13	20	0.11
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD21	20	0.11
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD22	20	0.11
(1,474)	1:99:A:VAL:HG13	1:142:A:LEU:HD23	20	0.11
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD11	20	0.11
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD12	20	0.11
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD13	20	0.11
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD21	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD22	20	0.11
(1,474)	1:99:A:VAL:HG21	1:142:A:LEU:HD23	20	0.11
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD11	20	0.11
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD12	20	0.11
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD13	20	0.11
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD21	20	0.11
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD22	20	0.11
(1,474)	1:99:A:VAL:HG22	1:142:A:LEU:HD23	20	0.11
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD11	20	0.11
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD12	20	0.11
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD13	20	0.11
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD21	20	0.11
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD22	20	0.11
(1,474)	1:99:A:VAL:HG23	1:142:A:LEU:HD23	20	0.11
(1,473)	1:99:A:VAL:HG11	1:104:A:ILE:H	5	0.11
(1,473)	1:99:A:VAL:HG12	1:104:A:ILE:H	5	0.11
(1,473)	1:99:A:VAL:HG13	1:104:A:ILE:H	5	0.11
(1,473)	1:99:A:VAL:HG21	1:104:A:ILE:H	5	0.11
(1,473)	1:99:A:VAL:HG22	1:104:A:ILE:H	5	0.11
(1,473)	1:99:A:VAL:HG23	1:104:A:ILE:H	5	0.11
(1,455)	1:72:A:LEU:HD11	1:114:A:LEU:H	18	0.11
(1,455)	1:72:A:LEU:HD12	1:114:A:LEU:H	18	0.11
(1,455)	1:72:A:LEU:HD13	1:114:A:LEU:H	18	0.11
(1,455)	1:72:A:LEU:HD21	1:114:A:LEU:H	18	0.11
(1,455)	1:72:A:LEU:HD22	1:114:A:LEU:H	18	0.11
(1,455)	1:72:A:LEU:HD23	1:114:A:LEU:H	18	0.11
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG11	3	0.11
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG12	3	0.11
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG13	3	0.11
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG21	3	0.11
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG22	3	0.11
(1,439)	1:53:A:ALA:H	1:156:A:VAL:HG23	3	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG11	6	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG12	6	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG13	6	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG21	6	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG22	6	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG23	6	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG11	6	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG12	6	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG13	6	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG21	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG22	6	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG23	6	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG11	6	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG12	6	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG13	6	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG21	6	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG22	6	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG23	6	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG11	6	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG12	6	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG13	6	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG21	6	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG22	6	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG23	6	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG11	6	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG12	6	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG13	6	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG21	6	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG22	6	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG23	6	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG11	6	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG12	6	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG13	6	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG21	6	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG22	6	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG23	6	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG11	20	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG12	20	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG13	20	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG21	20	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG22	20	0.11
(1,427)	1:21:A:LEU:HD11	1:127:A:VAL:HG23	20	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG11	20	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG12	20	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG13	20	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG21	20	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG22	20	0.11
(1,427)	1:21:A:LEU:HD12	1:127:A:VAL:HG23	20	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG11	20	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG12	20	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG13	20	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG21	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG22	20	0.11
(1,427)	1:21:A:LEU:HD13	1:127:A:VAL:HG23	20	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG11	20	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG12	20	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG13	20	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG21	20	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG22	20	0.11
(1,427)	1:21:A:LEU:HD21	1:127:A:VAL:HG23	20	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG11	20	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG12	20	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG13	20	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG21	20	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG22	20	0.11
(1,427)	1:21:A:LEU:HD22	1:127:A:VAL:HG23	20	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG11	20	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG12	20	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG13	20	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG21	20	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG22	20	0.11
(1,427)	1:21:A:LEU:HD23	1:127:A:VAL:HG23	20	0.11
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	10	0.11
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	10	0.11
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	10	0.11
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	10	0.11
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	10	0.11
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	10	0.11
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD21	7	0.11
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD22	7	0.11
(1,376)	1:72:A:LEU:HD21	1:94:A:LEU:HD23	7	0.11
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD21	7	0.11
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD22	7	0.11
(1,376)	1:72:A:LEU:HD22	1:94:A:LEU:HD23	7	0.11
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD21	7	0.11
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD22	7	0.11
(1,376)	1:72:A:LEU:HD23	1:94:A:LEU:HD23	7	0.11
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD21	5	0.11
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD22	5	0.11
(1,359)	1:104:A:ILE:HD11	1:142:A:LEU:HD23	5	0.11
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD21	5	0.11
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD22	5	0.11
(1,359)	1:104:A:ILE:HD12	1:142:A:LEU:HD23	5	0.11
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD21	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD22	5	0.11
(1,359)	1:104:A:ILE:HD13	1:142:A:LEU:HD23	5	0.11
(1,331)	1:13:A:VAL:HG11	1:136:A:THR:H	2	0.11
(1,331)	1:13:A:VAL:HG12	1:136:A:THR:H	2	0.11
(1,331)	1:13:A:VAL:HG13	1:136:A:THR:H	2	0.11
(1,292)	1:146:A:ILE:HD11	1:152:A:TRP:H	12	0.11
(1,292)	1:146:A:ILE:HD12	1:152:A:TRP:H	12	0.11
(1,292)	1:146:A:ILE:HD13	1:152:A:TRP:H	12	0.11
(1,278)	1:133:A:TRP:H	1:133:A:TRP:HE1	16	0.11
(1,268)	1:162:A:ASN:H	1:163:A:ALA:H	6	0.11
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	13	0.11
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	18	0.11
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	15	0.11
(1,248)	1:121:A:LYS:H	1:124:A:GLN:H	16	0.11
(1,234)	1:116:A:VAL:H	1:117:A:GLU:H	9	0.11
(1,231)	1:66:A:ARG:H	1:67:A:ARG:H	17	0.11
(1,211)	1:32:A:SER:H	1:35:A:GLU:H	10	0.11
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	3	0.11
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	5	0.11
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	15	0.11
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	20	0.11
(1,191)	1:101:A:TRP:H	1:102:A:GLY:H	11	0.11
(1,190)	1:102:A:GLY:H	1:106:A:ALA:H	1	0.11
(1,189)	1:69:A:PHE:H	1:72:A:LEU:H	6	0.11
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	13	0.11
(1,187)	1:110:A:PHE:H	1:113:A:ALA:H	14	0.11
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	7	0.11
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	15	0.11
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	17	0.11
(1,150)	1:126:A:LEU:H	1:129:A:ARG:H	6	0.11
(1,149)	1:129:A:ARG:H	1:131:A:ALA:H	12	0.11
(1,147)	1:163:A:ALA:H	1:164:A:ALA:H	20	0.11
(1,130)	1:119:A:VAL:H	1:122:A:GLU:H	2	0.11
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	9	0.11
(1,124)	1:39:A:THR:H	1:40:A:GLU:H	1	0.11
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	15	0.11
(1,120)	1:54:A:LEU:H	1:56:A:GLU:H	17	0.11
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	7	0.11
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	10	0.11
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	6	0.11
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	20	0.11
(1,95)	1:89:A:GLN:H	1:91:A:VAL:H	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:109:A:SER:H	1:111:A:GLY:H	19	0.11
(1,90)	1:8:A:SER:H	1:10:A:ARG:H	10	0.11
(1,90)	1:8:A:SER:H	1:10:A:ARG:H	18	0.11
(1,83)	1:152:A:TRP:H	1:154:A:THR:H	16	0.11
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	14	0.11
(1,73)	1:88:A:GLU:H	1:90:A:VAL:H	17	0.11
(1,68)	1:158:A:LEU:H	1:161:A:ASN:H	1	0.11
(1,60)	1:13:A:VAL:H	1:16:A:PHE:H	13	0.11
(1,55)	1:15:A:ASP:H	1:17:A:LEU:H	18	0.11
(1,48)	1:120:A:ASP:H	1:122:A:GLU:H	17	0.11
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	19	0.11
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	8	0.11
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	10	0.11
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	20	0.11
(1,22)	1:105:A:VAL:H	1:107:A:PHE:H	6	0.11
(1,21)	1:43:A:GLU:H	1:44:A:GLY:H	4	0.11
(1,19)	1:30:A:GLN:H	1:32:A:SER:H	16	0.11
(1,14)	1:92:A:ASN:H	1:94:A:LEU:H	18	0.11
(1,12)	1:51:A:LYS:H	1:53:A:ALA:H	2	0.11
(1,6)	1:63:A:LEU:H	1:65:A:TYR:H	7	0.11
(1,5)	1:65:A:TYR:H	1:66:A:ARG:H	19	0.11
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD11	16	0.1
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD12	16	0.1
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD13	16	0.1
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD21	16	0.1
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD22	16	0.1
(1,503)	1:138:A:LEU:H	1:142:A:LEU:HD23	16	0.1
(1,500)	1:127:A:VAL:HG11	1:130:A:ILE:HD11	12	0.1
(1,500)	1:127:A:VAL:HG11	1:130:A:ILE:HD12	12	0.1
(1,500)	1:127:A:VAL:HG11	1:130:A:ILE:HD13	12	0.1
(1,500)	1:127:A:VAL:HG12	1:130:A:ILE:HD11	12	0.1
(1,500)	1:127:A:VAL:HG12	1:130:A:ILE:HD12	12	0.1
(1,500)	1:127:A:VAL:HG12	1:130:A:ILE:HD13	12	0.1
(1,500)	1:127:A:VAL:HG13	1:130:A:ILE:HD11	12	0.1
(1,500)	1:127:A:VAL:HG13	1:130:A:ILE:HD12	12	0.1
(1,500)	1:127:A:VAL:HG13	1:130:A:ILE:HD13	12	0.1
(1,500)	1:127:A:VAL:HG21	1:130:A:ILE:HD11	12	0.1
(1,500)	1:127:A:VAL:HG21	1:130:A:ILE:HD12	12	0.1
(1,500)	1:127:A:VAL:HG21	1:130:A:ILE:HD13	12	0.1
(1,500)	1:127:A:VAL:HG22	1:130:A:ILE:HD11	12	0.1
(1,500)	1:127:A:VAL:HG22	1:130:A:ILE:HD12	12	0.1
(1,500)	1:127:A:VAL:HG22	1:130:A:ILE:HD13	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,500)	1:127:A:VAL:HG23	1:130:A:ILE:HD11	12	0.1
(1,500)	1:127:A:VAL:HG23	1:130:A:ILE:HD12	12	0.1
(1,500)	1:127:A:VAL:HG23	1:130:A:ILE:HD13	12	0.1
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG11	18	0.1
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG12	18	0.1
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG13	18	0.1
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG21	18	0.1
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG22	18	0.1
(1,486)	1:119:A:VAL:HG11	1:127:A:VAL:HG23	18	0.1
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG11	18	0.1
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG12	18	0.1
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG13	18	0.1
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG21	18	0.1
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG22	18	0.1
(1,486)	1:119:A:VAL:HG12	1:127:A:VAL:HG23	18	0.1
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG11	18	0.1
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG12	18	0.1
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG13	18	0.1
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG21	18	0.1
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG22	18	0.1
(1,486)	1:119:A:VAL:HG13	1:127:A:VAL:HG23	18	0.1
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG11	18	0.1
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG12	18	0.1
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG13	18	0.1
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG21	18	0.1
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG22	18	0.1
(1,486)	1:119:A:VAL:HG21	1:127:A:VAL:HG23	18	0.1
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG11	18	0.1
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG12	18	0.1
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG13	18	0.1
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG21	18	0.1
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG22	18	0.1
(1,486)	1:119:A:VAL:HG22	1:127:A:VAL:HG23	18	0.1
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG11	18	0.1
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG12	18	0.1
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG13	18	0.1
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG21	18	0.1
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG22	18	0.1
(1,486)	1:119:A:VAL:HG23	1:127:A:VAL:HG23	18	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	9	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	9	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	9	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	9	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	9	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	9	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	9	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	9	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	9	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	9	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	9	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	9	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	9	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	9	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	9	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	9	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	9	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	9	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	9	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	9	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	9	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	9	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	9	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	9	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	9	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	9	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	9	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	9	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	9	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	9	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	9	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	9	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	9	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	9	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	9	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD11	11	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD12	11	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD13	11	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD21	11	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD22	11	0.1
(1,433)	1:50:A:VAL:HG11	1:54:A:LEU:HD23	11	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD11	11	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD12	11	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD13	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD21	11	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD22	11	0.1
(1,433)	1:50:A:VAL:HG12	1:54:A:LEU:HD23	11	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD11	11	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD12	11	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD13	11	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD21	11	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD22	11	0.1
(1,433)	1:50:A:VAL:HG13	1:54:A:LEU:HD23	11	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD11	11	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD12	11	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD13	11	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD21	11	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD22	11	0.1
(1,433)	1:50:A:VAL:HG21	1:54:A:LEU:HD23	11	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD11	11	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD12	11	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD13	11	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD21	11	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD22	11	0.1
(1,433)	1:50:A:VAL:HG22	1:54:A:LEU:HD23	11	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD11	11	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD12	11	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD13	11	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD21	11	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD22	11	0.1
(1,433)	1:50:A:VAL:HG23	1:54:A:LEU:HD23	11	0.1
(1,379)	1:17:A:LEU:HD11	1:114:A:LEU:H	6	0.1
(1,379)	1:17:A:LEU:HD12	1:114:A:LEU:H	6	0.1
(1,379)	1:17:A:LEU:HD13	1:114:A:LEU:H	6	0.1
(1,379)	1:17:A:LEU:HD21	1:114:A:LEU:H	6	0.1
(1,379)	1:17:A:LEU:HD22	1:114:A:LEU:H	6	0.1
(1,379)	1:17:A:LEU:HD23	1:114:A:LEU:H	6	0.1
(1,369)	1:78:A:ILE:HD11	1:126:A:LEU:HD21	13	0.1
(1,369)	1:78:A:ILE:HD11	1:126:A:LEU:HD22	13	0.1
(1,369)	1:78:A:ILE:HD11	1:126:A:LEU:HD23	13	0.1
(1,369)	1:78:A:ILE:HD12	1:126:A:LEU:HD21	13	0.1
(1,369)	1:78:A:ILE:HD12	1:126:A:LEU:HD22	13	0.1
(1,369)	1:78:A:ILE:HD12	1:126:A:LEU:HD23	13	0.1
(1,369)	1:78:A:ILE:HD13	1:126:A:LEU:HD21	13	0.1
(1,369)	1:78:A:ILE:HD13	1:126:A:LEU:HD22	13	0.1
(1,369)	1:78:A:ILE:HD13	1:126:A:LEU:HD23	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:12:A:LEU:HD21	1:51:A:LYS:H	13	0.1
(1,338)	1:12:A:LEU:HD22	1:51:A:LYS:H	13	0.1
(1,338)	1:12:A:LEU:HD23	1:51:A:LYS:H	13	0.1
(1,302)	1:104:A:ILE:HD11	1:146:A:ILE:H	1	0.1
(1,302)	1:104:A:ILE:HD12	1:146:A:ILE:H	1	0.1
(1,302)	1:104:A:ILE:HD13	1:146:A:ILE:H	1	0.1
(1,285)	1:17:A:LEU:HD11	1:132:A:ALA:H	16	0.1
(1,285)	1:17:A:LEU:HD12	1:132:A:ALA:H	16	0.1
(1,285)	1:17:A:LEU:HD13	1:132:A:ALA:H	16	0.1
(1,285)	1:17:A:LEU:HD21	1:132:A:ALA:H	16	0.1
(1,285)	1:17:A:LEU:HD22	1:132:A:ALA:H	16	0.1
(1,285)	1:17:A:LEU:HD23	1:132:A:ALA:H	16	0.1
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	9	0.1
(1,271)	1:18:A:SER:H	1:20:A:LYS:H	20	0.1
(1,268)	1:162:A:ASN:H	1:163:A:ALA:H	10	0.1
(1,268)	1:162:A:ASN:H	1:163:A:ALA:H	11	0.1
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	6	0.1
(1,261)	1:110:A:PHE:H	1:112:A:GLY:H	11	0.1
(1,231)	1:66:A:ARG:H	1:67:A:ARG:H	8	0.1
(1,216)	1:24:A:LYS:H	1:26:A:TYR:H	17	0.1
(1,212)	1:99:A:VAL:H	1:102:A:GLY:H	16	0.1
(1,209)	1:103:A:ARG:H	1:106:A:ALA:H	3	0.1
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	10	0.1
(1,202)	1:54:A:LEU:H	1:57:A:ALA:H	20	0.1
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	1	0.1
(1,196)	1:50:A:VAL:H	1:51:A:LYS:H	12	0.1
(1,182)	1:73:A:THR:H	1:75:A:GLN:H	11	0.1
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	12	0.1
(1,175)	1:135:A:ALA:H	1:137:A:TYR:H	13	0.1
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	4	0.1
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	5	0.1
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	14	0.1
(1,168)	1:48:A:GLU:H	1:50:A:VAL:H	16	0.1
(1,162)	1:126:A:LEU:H	1:127:A:VAL:H	9	0.1
(1,159)	1:101:A:TRP:H	1:104:A:ILE:H	8	0.1
(1,129)	1:93:A:GLU:H	1:95:A:PHE:H	11	0.1
(1,123)	1:75:A:GLN:H	1:77:A:HIS:H	7	0.1
(1,116)	1:163:A:ALA:H	1:166:A:GLU:H	10	0.1
(1,115)	1:107:A:PHE:H	1:109:A:SER:H	7	0.1
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	5	0.1
(1,107)	1:145:A:TRP:H	1:146:A:ILE:H	19	0.1
(1,98)	1:157:A:GLU:H	1:159:A:TYR:H	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:27:A:SER:H	1:28:A:TRP:H	9	0.1
(1,37)	1:133:A:TRP:H	1:135:A:ALA:H	1	0.1
(1,31)	1:136:A:THR:H	1:138:A:LEU:H	13	0.1
(1,29)	1:135:A:ALA:H	1:138:A:LEU:H	7	0.1
(1,21)	1:43:A:GLU:H	1:44:A:GLY:H	7	0.1

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

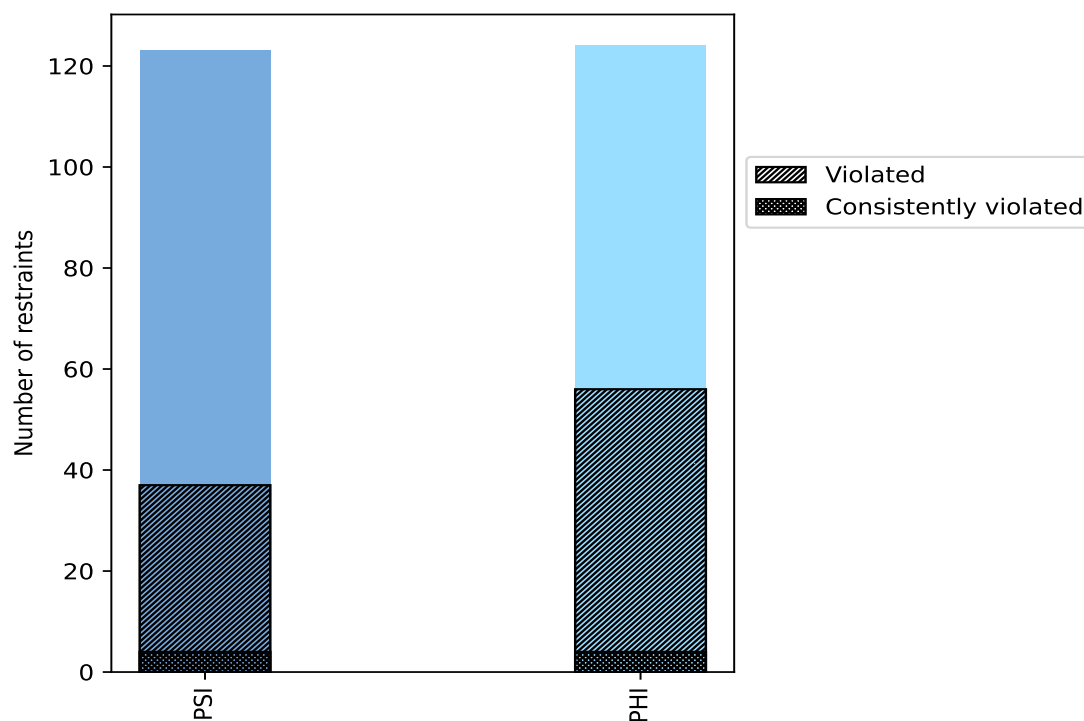
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	123	49.8	37	30.1	15.0	4	3.3	1.6
PHI	124	50.2	56	45.2	22.7	4	3.2	1.6
Total	247	100.0	93	37.7	37.7	8	3.2	3.2

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 [i](#)



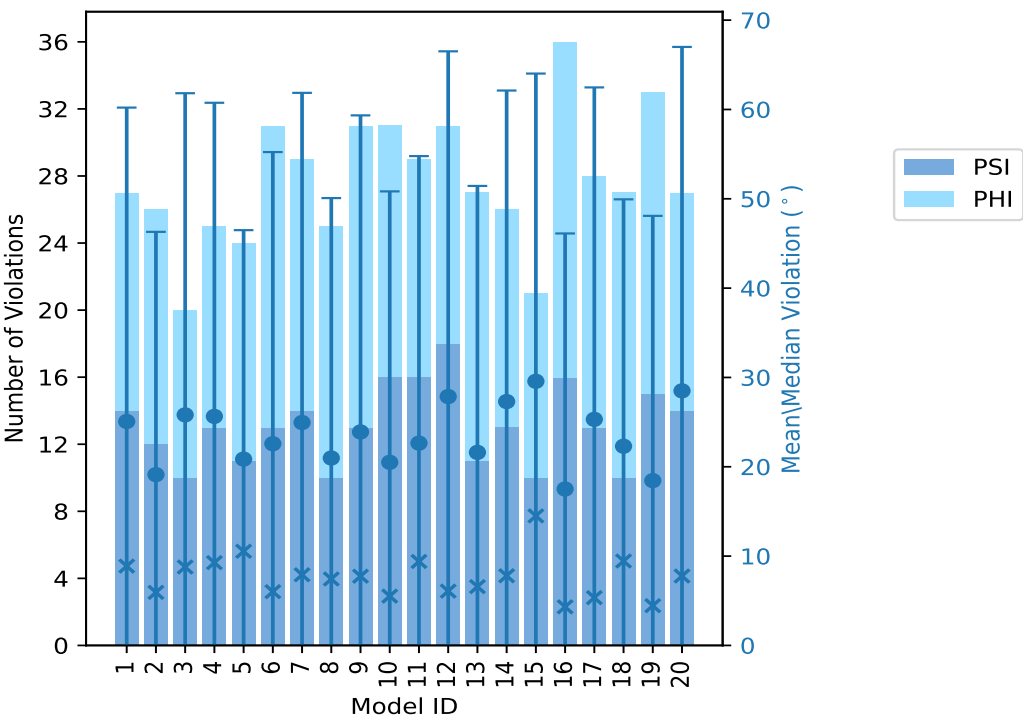
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	14	13	27	25.07	141.58	35.14	8.88
2	12	14	26	19.12	123.92	27.18	5.94
3	10	10	20	25.81	155.42	36.01	8.78
4	13	12	25	25.64	134.69	35.11	9.27
5	11	13	24	20.86	110.43	25.63	10.54
6	13	18	31	22.58	114.08	32.65	6.02
7	14	15	29	24.95	155.27	36.91	7.91
8	10	15	25	20.98	122.56	29.1	7.44
9	13	18	31	23.9	131.97	35.44	7.75
10	16	15	31	20.5	130.26	30.33	5.52
11	16	13	29	22.65	125.38	32.13	9.4
12	18	13	31	27.86	124.29	38.65	6.08
13	11	16	27	21.61	122.8	29.83	6.58
14	13	13	26	27.3	119.11	34.82	7.8
15	10	11	21	29.57	122.71	34.45	14.5
16	16	20	36	17.51	150.89	28.61	4.32
17	13	15	28	25.31	148.02	37.16	5.35
18	10	17	27	22.3	93.04	27.64	9.45
19	15	18	33	18.45	118.37	29.64	4.45
20	14	13	27	28.5	128.96	38.5	7.77

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	%
12	18	30	1	5.0
1	10	11	2	10.0
3	7	10	3	15.0
1	5	6	4	20.0
4	2	6	5	25.0
1	0	1	6	30.0
3	2	5	7	35.0
2	0	2	8	40.0
0	3	3	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

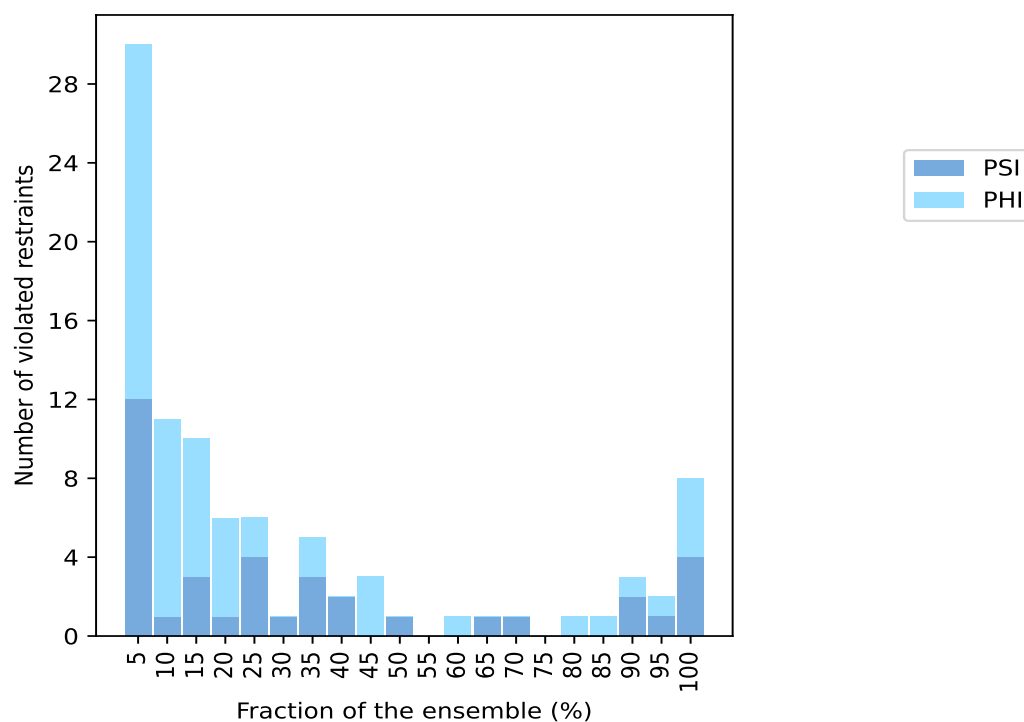
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	1	1	12	60.0
1	0	1	13	65.0
1	0	1	14	70.0
0	0	0	15	75.0
0	1	1	16	80.0
0	1	1	17	85.0
2	1	3	18	90.0
1	1	2	19	95.0
4	4	8	20	100.0

¹ Number of models with violations

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

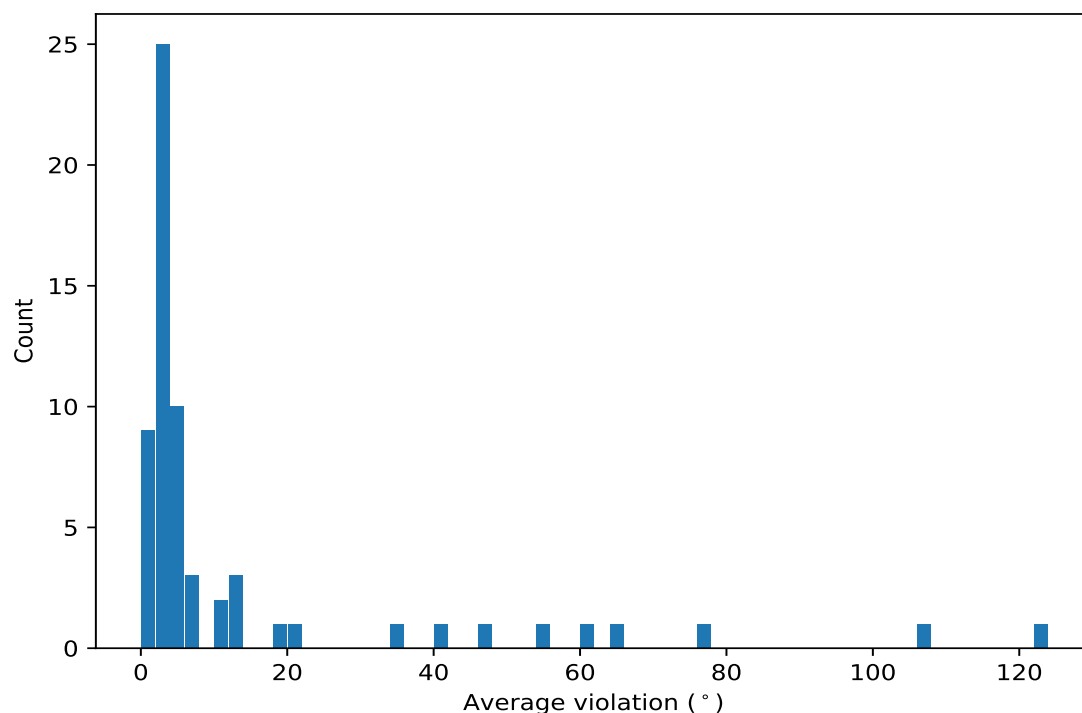


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	20	60.19	2.1	60.89
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	20	54.27	32.7	45.28
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	20	46.92	4.5	45.82
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	20	34.15	2.01	33.88
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	20	19.65	2.58	19.34
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	20	13.55	2.0	13.2
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	20	10.25	2.67	10.07
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	20	6.37	1.44	6.62
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	19	77.36	23.31	83.66
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	19	5.46	3.91	3.98
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	18	123.87	31.82	123.38
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	18	40.32	18.74	35.75
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	18	12.09	8.32	9.02
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	17	65.46	37.71	58.43
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	16	7.15	3.71	6.26
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	14	2.11	0.61	1.98
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	13	6.84	1.6	6.83
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	12	3.15	0.85	2.88
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	10	2.18	1.32	1.74
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	9	107.18	19.85	109.96

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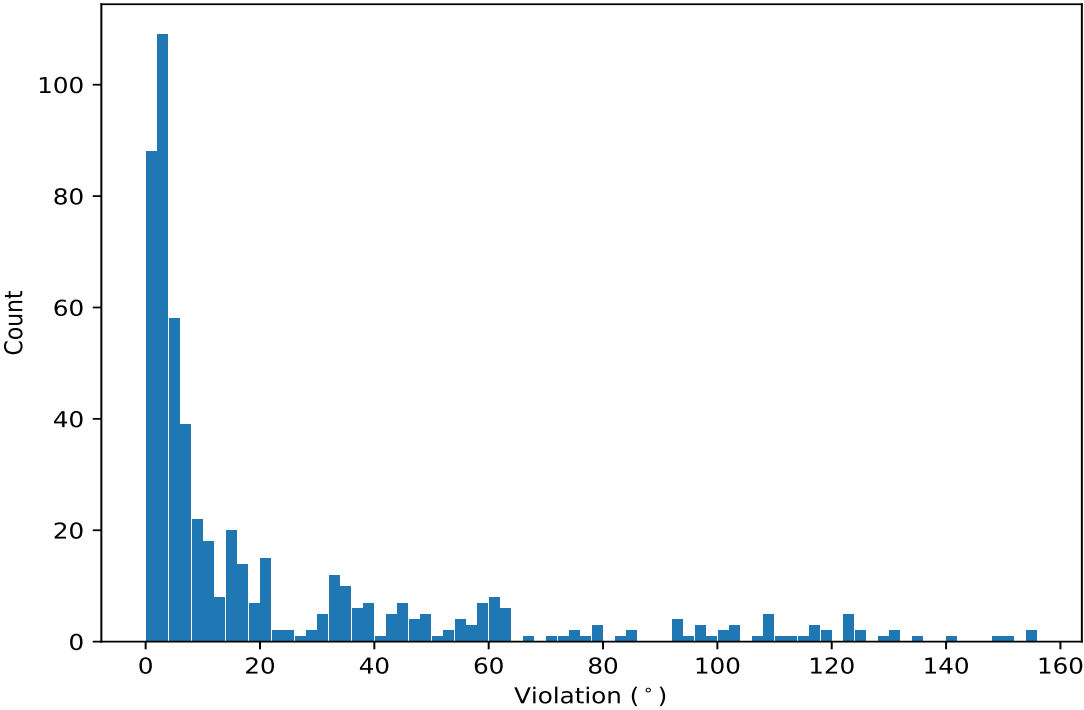
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	9	4.33	2.28	3.38
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	9	3.95	3.03	2.42
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	8	13.4	6.83	15.62
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	8	3.16	1.23	2.73
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	7	20.63	0.71	20.66
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	7	4.65	2.61	3.39
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	7	3.73	1.81	2.93
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	7	2.55	0.95	2.49
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	7	1.87	0.77	1.33
(1,172)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:MET:N	6	3.72	1.43	2.96
(1,52)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ASP:N	5	4.71	2.97	3.15
(1,53)	1:45:A:THR:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	5	4.42	1.43	4.32
(1,178)	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	1:126:A:LEU:N	5	4.32	1.64	5.09
(1,235)	1:162:A:ASN:C	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	5	3.95	1.3	4.28
(1,44)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:TRP:N	5	3.4	1.84	2.61
(1,108)	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	1:85:A:GLN:N	5	2.76	0.9	2.35
(1,171)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	4	5.95	2.12	5.38
(1,219)	1:148:A:GLU:C	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	4	3.6	1.34	3.82
(1,175)	1:123:A:MET:C	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	4	3.24	3.06	1.74
(1,183)	1:127:A:VAL:C	1:128:A:SER:N	1:128:A:SER:CA	1:128:A:SER:C	4	2.92	1.33	3.01
(1,229)	1:155:A:PHE:C	1:156:A:VAL:N	1:156:A:VAL:CA	1:156:A:VAL:C	4	1.53	0.38	1.54
(1,98)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:LEU:N	4	1.5	0.21	1.49
(1,176)	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	1:125:A:VAL:N	3	10.71	5.85	14.22
(1,49)	1:29:A:SER:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	3	4.27	1.49	3.92
(1,207)	1:139:A:ASN:C	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	3	3.12	1.6	2.28
(1,62)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:GLN:N	3	2.65	1.2	2.79
(1,37)	1:21:A:LEU:C	1:22:A:SER:N	1:22:A:SER:CA	1:22:A:SER:C	3	2.43	0.59	2.08
(1,115)	1:88:A:GLU:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	3	2.37	0.44	2.6
(1,186)	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	1:130:A:ILE:N	3	2.27	1.06	2.0
(1,107)	1:83:A:ALA:C	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	3	2.01	0.53	2.22
(1,51)	1:31:A:PHE:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	3	1.98	0.42	1.98
(1,217)	1:147:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	3	1.68	0.55	1.58
(1,160)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:GLU:N	2	4.76	0.08	4.76
(1,113)	1:87:A:PHE:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	2	4.26	1.12	4.26
(1,93)	1:68:A:ALA:C	1:69:A:PHE:N	1:69:A:PHE:CA	1:69:A:PHE:C	2	3.2	1.1	3.2
(1,127)	1:94:A:LEU:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	2	2.33	0.55	2.33
(1,71)	1:55:A:ARG:C	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	2	2.26	0.86	2.26
(1,181)	1:126:A:LEU:C	1:127:A:VAL:N	1:127:A:VAL:CA	1:127:A:VAL:C	2	2.12	0.14	2.12
(1,189)	1:130:A:ILE:C	1:131:A:ALA:N	1:131:A:ALA:CA	1:131:A:ALA:C	2	2.07	0.98	2.07
(1,101)	1:72:A:LEU:C	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	2	1.9	0.31	1.9
(1,179)	1:125:A:VAL:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	2	1.84	0.01	1.84
(1,165)	1:118:A:SER:C	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	2	1.62	0.17	1.62
(1,123)	1:92:A:ASN:C	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	2	1.6	0.17	1.6

¹ Number of violated models, ²Standard 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 (°)
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	3	155.42
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	7	155.27
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	16	150.89
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	17	148.02
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	1	141.58
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	4	134.69
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	9	131.97
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	10	130.26
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	20	128.96
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	11	125.38
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	12	124.29
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	2	123.92
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	12	122.85
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	13	122.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	15	122.71
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	8	122.56
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	14	119.11
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	19	118.37
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	20	117.91
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	20	117.34
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	19	116.27
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	6	114.08
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	9	112.62
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	5	110.43
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	7	109.96
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	6	109.96
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	15	109.64
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1	109.56
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	9	108.48
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	12	107.58
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	14	103.25
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	10	102.5
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	4	102.38
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	17	101.1
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	6	100.61
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	7	98.3
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	14	97.32
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	11	96.41
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	17	96.15
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	12	94.62
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	18	93.04
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	4	92.83
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	11	92.75
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	18	92.03
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1	85.06
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	8	84.19
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	13	83.66
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	14	79.1
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	12	78.6
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	18	78.33
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	20	77.16
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	12	75.86
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	9	75.14
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	15	73.48
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	3	70.41
(1,177)	1:124:A:GLN:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	17	66.43
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	16	63.5
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	14	63.48
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	18	63.27
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	16	63.21
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	5	62.64
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	4	62.0
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	19	61.63
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1	61.56
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	20	61.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	13	61.11
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	3	60.98
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	6	60.93
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	7	60.85
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	10	60.27
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	10	59.49
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	2	59.37
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	11	59.01
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	15	58.91
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	2	58.43
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	5	58.33
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	17	58.02
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	9	57.26
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	8	57.16
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	6	56.03
(1,213)	1:145:A:TRP:C	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	12	55.94
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	13	55.66
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	20	55.47
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1	54.98
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	19	53.64
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	17	52.53
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	11	51.52
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	8	49.59
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	3	48.83
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	17	48.65
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	7	48.59
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	16	48.16
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	13	47.69
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	20	47.19
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	18	46.65
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	9	46.12
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	11	45.65
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	6	45.62
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	2	45.51
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	14	44.92
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	4	44.57
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	5	44.54
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	16	44.47
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	6	43.97
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	19	43.88
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	12	42.86
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	14	42.51
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	15	42.23
(1,133)	1:101:A:TRP:C	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	13	41.52
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	15	39.82
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	7	39.68
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	15	39.22
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	10	38.89
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	13	38.76
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	10	38.59
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	7	38.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	4	37.77
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	10	36.58
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	5	36.22
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	19	36.21
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	2	36.12
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	11	36.11
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	17	35.57
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	16	35.39
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	8	35.08
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	9	34.77
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	1	34.61
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	12	34.49
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	9	34.35
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	13	34.28
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	3	34.22
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	3	34.17
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	20	33.92
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	6	33.83
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	5	33.83
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	16	33.45
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	19	33.38
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	15	33.36
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	14	33.23
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	2	33.18
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	18	32.95
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	18	32.65
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	4	32.59
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	16	32.14
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	18	31.97
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	7	31.81
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	8	30.99
(1,209)	1:140:A:ASP:C	1:141:A:HIS:N	1:141:A:HIS:CA	1:141:A:HIS:C	1	30.97
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	3	30.53
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	10	29.14
(1,245)	1:175:A:GLU:C	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	5	28.13
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	8	27.91
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	10	25.48
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	16	24.46
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	2	23.06
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	13	22.57
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	20	21.93
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	19	21.68
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	16	21.44
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1	21.4
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	15	21.16
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	10	21.07
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	19	21.03
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	6	20.84
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	6	20.8
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	4	20.66
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	2	20.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	2	20.38
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	7	20.35
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	4	20.13
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	11	20.07
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	9	19.83
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	12	19.45
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	18	19.22
(1,234)	1:158:A:LEU:N	1:158:A:LEU:CA	1:158:A:LEU:C	1:159:A:TYR:N	1	19.1
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	14	19.06
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	1	19.05
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	15	18.77
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	17	17.91
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	17	17.85
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	3	17.72
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	18	17.72
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	7	17.64
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	5	17.6
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	8	17.48
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	5	17.43
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	16	16.98
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	6	16.92
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	14	16.63
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	4	16.42
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	11	16.27
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	16	16.09
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	1	15.6
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	2	15.59
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	11	15.45
(1,176)	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	1:125:A:VAL:N	12	15.44
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	8	15.42
(1,173)	1:122:A:GLU:C	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	8	15.27
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	13	14.96
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	14	14.96
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	8	14.96
(1,204)	1:138:A:LEU:N	1:138:A:LEU:CA	1:138:A:LEU:C	1:139:A:ASN:N	7	14.95
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	20	14.69
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	8	14.59
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	15	14.5
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	19	14.42
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	20	14.34
(1,176)	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	1:125:A:VAL:N	9	14.22
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	4	14.2
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	1	14.07
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	11	14.04
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	10	14.03
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	20	13.96
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	5	13.91
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	17	13.71
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	5	13.69
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	12	12.7
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	9	12.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	14	12.34
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	18	12.1
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	3	11.97
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	18	11.96
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	7	11.9
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	19	11.89
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	5	11.79
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	20	11.69
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	4	11.51
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	7	11.36
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	6	11.29
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	16	11.2
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	15	10.86
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	18	10.84
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	3	10.72
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	2	10.55
(1,208)	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	1:141:A:HIS:N	11	10.33
(1,52)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ASP:N	10	10.3
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	1	10.11
(1,43)	1:26:A:TYR:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	19	10.06
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	7	9.99
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	11	9.66
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	12	9.63
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	19	9.59
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	11	9.55
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	18	9.45
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	11	9.4
(1,171)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	9	9.37
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	5	9.29
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	4	9.27
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	15	9.18
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	9	9.1
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	6	8.98
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	12	8.91
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	1	8.88
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	9	8.73
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	13	8.53
(1,175)	1:123:A:MET:C	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	6	8.49
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	18	8.3
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	18	8.25
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	12	8.12
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	13	8.08
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	14	7.96
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	9	7.92
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	7	7.91
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	20	7.77
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	1	7.76
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	9	7.75
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	5	7.7
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	13	7.65
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	14	7.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	19	7.61
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	10	7.5
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	11	7.47
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	8	7.44
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	5	7.31
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	16	7.24
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	16	7.19
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	5	7.09
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	1	7.01
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	10	7.0
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	9	6.89
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	2	6.85
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	3	6.83
(1,44)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:TRP:N	3	6.79
(1,53)	1:45:A:THR:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	9	6.66
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	13	6.58
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	20	6.51
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	6	6.5
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	17	6.43
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	14	6.39
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	4	6.36
(1,172)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:MET:N	4	6.33
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	10	6.31
(1,178)	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	1:126:A:LEU:N	14	6.26
(1,174)	1:123:A:MET:N	1:123:A:MET:CA	1:123:A:MET:C	1:124:A:GLN:N	19	6.24
(1,49)	1:29:A:SER:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	7	6.24
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	12	6.08
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	20	6.08
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	2	6.03
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	6	6.02
(1,85)	1:62:A:GLU:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	7	5.97
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	20	5.96
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	3	5.95
(1,171)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	20	5.88
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	5	5.87
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	2	5.85
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	1	5.78
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	16	5.77
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	9	5.77
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	6	5.76
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	14	5.69
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	17	5.61
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	17	5.57
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	4	5.56
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	16	5.53
(1,235)	1:162:A:ASN:C	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	10	5.52
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	8	5.5
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	7	5.45
(1,113)	1:87:A:PHE:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	10	5.38
(1,178)	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	1:126:A:LEU:N	11	5.37
(1,207)	1:139:A:ASN:C	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	16	5.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	19	5.35
(1,53)	1:45:A:THR:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	1	5.2
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	12	5.19
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	17	5.12
(1,178)	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	1:126:A:LEU:N	18	5.09
(1,52)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ASP:N	11	5.08
(1,219)	1:148:A:GLU:C	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	18	5.06
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	14	5.02
(1,172)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:MET:N	2	4.94
(1,237)	1:163:A:ALA:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	17	4.92
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	3	4.89
(1,171)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	17	4.89
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	14	4.86
(1,160)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:GLU:N	18	4.85
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	15	4.83
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	15	4.8
(1,216)	1:147:A:GLN:N	1:147:A:GLN:CA	1:147:A:GLN:C	1:148:A:GLU:N	9	4.77
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	9	4.74
(1,160)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:GLU:N	1	4.68
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	7	4.66
(1,219)	1:148:A:GLU:C	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	3	4.64
(1,246)	1:176:A:HIS:N	1:176:A:HIS:CA	1:176:A:HIS:C	1:177:A:HIS:N	18	4.46
(1,183)	1:127:A:VAL:C	1:128:A:SER:N	1:128:A:SER:CA	1:128:A:SER:C	19	4.45
(1,235)	1:162:A:ASN:C	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	15	4.42
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	7	4.42
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	8	4.34
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	1	4.32
(1,53)	1:45:A:THR:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	4	4.32
(1,93)	1:68:A:ALA:C	1:69:A:PHE:N	1:69:A:PHE:CA	1:69:A:PHE:C	20	4.3
(1,235)	1:162:A:ASN:C	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	11	4.28
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	12	4.26
(1,108)	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	1:85:A:GLN:N	12	4.12
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	12	4.1
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	10	4.07
(1,180)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:VAL:N	17	4.05
(1,62)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:GLN:N	10	4.05
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	14	4.03
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	15	3.99
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	2	3.98
(1,235)	1:162:A:ASN:C	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	4	3.94
(1,183)	1:127:A:VAL:C	1:128:A:SER:N	1:128:A:SER:CA	1:128:A:SER:C	14	3.94
(1,49)	1:29:A:SER:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	2	3.92
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	19	3.9
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	11	3.78
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	7	3.77
(1,200)	1:136:A:THR:N	1:136:A:THR:CA	1:136:A:THR:C	1:137:A:TYR:N	15	3.72
(1,186)	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	1:130:A:ILE:N	12	3.68
(1,171)	1:121:A:LYS:C	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	12	3.67
(1,44)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:TRP:N	10	3.61
(1,155)	1:113:A:ALA:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	14	3.58
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	10	3.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,108)	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	1:85:A:GLN:N	3	3.48
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	20	3.4
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	12	3.39
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	2	3.39
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	3	3.38
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	16	3.29
(1,170)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:GLU:N	12	3.28
(1,53)	1:45:A:THR:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	8	3.27
(1,37)	1:21:A:LEU:C	1:22:A:SER:N	1:22:A:SER:CA	1:22:A:SER:C	4	3.27
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	18	3.27
(1,172)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:MET:N	8	3.26
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	19	3.24
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	19	3.21
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	13	3.19
(1,113)	1:87:A:PHE:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	13	3.15
(1,52)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ASP:N	16	3.15
(1,42)	1:26:A:TYR:N	1:26:A:TYR:CA	1:26:A:TYR:C	1:27:A:SER:N	9	3.14
(1,178)	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	1:126:A:LEU:N	12	3.13
(1,71)	1:55:A:ARG:C	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	9	3.13
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	7	3.11
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	20	3.1
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	7	3.1
(1,189)	1:130:A:ILE:C	1:131:A:ALA:N	1:131:A:ALA:CA	1:131:A:ALA:C	10	3.05
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	6	3.04
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	9	3.04
(1,24)	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	1:16:A:PHE:N	16	3.01
(1,219)	1:148:A:GLU:C	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	8	2.99
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	4	2.98
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	5	2.98
(1,158)	1:115:A:CYS:N	1:115:A:CYS:CA	1:115:A:CYS:C	1:116:A:VAL:N	11	2.96
(1,52)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ASP:N	1	2.96
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	13	2.94
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	10	2.93
(1,127)	1:94:A:LEU:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	10	2.88
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	11	2.84
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	1	2.82
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	10	2.81
(1,62)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:GLN:N	16	2.79
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	6	2.77
(1,131)	1:100:A:ASN:C	1:101:A:TRP:N	1:101:A:TRP:CA	1:101:A:TRP:C	16	2.77
(1,115)	1:88:A:GLU:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	13	2.76
(1,143)	1:107:A:PHE:C	1:108:A:PHE:N	1:108:A:PHE:CA	1:108:A:PHE:C	19	2.74
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	6	2.73
(1,105)	1:74:A:SER:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	16	2.71
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	16	2.67
(1,172)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:MET:N	1	2.65
(1,49)	1:29:A:SER:C	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	15	2.65
(1,53)	1:45:A:THR:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	13	2.63
(1,172)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:MET:N	20	2.62
(1,44)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:TRP:N	11	2.61
(1,115)	1:88:A:GLU:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	10	2.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	8	2.59
(1,44)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:TRP:N	12	2.59
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	2	2.58
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	14	2.58
(1,172)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:MET:N	16	2.55
(1,169)	1:120:A:ASP:C	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	18	2.54
(1,107)	1:83:A:ALA:C	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	2	2.54
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	5	2.52
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	13	2.49
(1,51)	1:31:A:PHE:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	2	2.49
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	8	2.49
(1,12)	1:9:A:ASN:N	1:9:A:ASN:CA	1:9:A:ASN:C	1:10:A:ARG:N	7	2.49
(1,176)	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	1:125:A:VAL:N	17	2.47
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	5	2.45
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	9	2.44
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	20	2.42
(1,217)	1:147:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	9	2.39
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	12	2.39
(1,108)	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	1:85:A:GLN:N	11	2.35
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	19	2.32
(1,207)	1:139:A:ASN:C	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	6	2.28
(1,99)	1:71:A:ASP:C	1:72:A:LEU:N	1:72:A:LEU:CA	1:72:A:LEU:C	13	2.26
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	6	2.25
(1,181)	1:126:A:LEU:C	1:127:A:VAL:N	1:127:A:VAL:CA	1:127:A:VAL:C	13	2.25
(1,92)	1:68:A:ALA:N	1:68:A:ALA:CA	1:68:A:ALA:C	1:69:A:PHE:N	14	2.25
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	1	2.24
(1,195)	1:133:A:TRP:C	1:134:A:MET:N	1:134:A:MET:CA	1:134:A:MET:C	6	2.24
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	3	2.22
(1,107)	1:83:A:ALA:C	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	16	2.22
(1,101)	1:72:A:LEU:C	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	16	2.21
(1,108)	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	1:85:A:GLN:N	17	2.16
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	4	2.15
(1,175)	1:123:A:MET:C	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	2	2.14
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	4	2.14
(1,93)	1:68:A:ALA:C	1:69:A:PHE:N	1:69:A:PHE:CA	1:69:A:PHE:C	19	2.1
(1,183)	1:127:A:VAL:C	1:128:A:SER:N	1:128:A:SER:CA	1:128:A:SER:C	6	2.09
(1,37)	1:21:A:LEU:C	1:22:A:SER:N	1:22:A:SER:CA	1:22:A:SER:C	12	2.08
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	5	2.06
(1,52)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:ASP:N	20	2.04
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	2	2.03
(1,161)	1:116:A:VAL:C	1:117:A:GLU:N	1:117:A:GLU:CA	1:117:A:GLU:C	19	2.02
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	11	2.02
(1,229)	1:155:A:PHE:C	1:156:A:VAL:N	1:156:A:VAL:CA	1:156:A:VAL:C	5	2.01
(1,186)	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	1:130:A:ILE:N	6	2.0
(1,181)	1:126:A:LEU:C	1:127:A:VAL:N	1:127:A:VAL:CA	1:127:A:VAL:C	6	1.98
(1,51)	1:31:A:PHE:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	10	1.98
(1,166)	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	1:120:A:ASP:N	19	1.97
(1,37)	1:21:A:LEU:C	1:22:A:SER:N	1:22:A:SER:CA	1:22:A:SER:C	14	1.95
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	4	1.92
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	11	1.92
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	13	1.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,223)	1:152:A:TRP:C	1:153:A:ASP:N	1:153:A:ASP:CA	1:153:A:ASP:C	1	1.89
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	9	1.88
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	3	1.87
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	1	1.86
(1,103)	1:73:A:THR:C	1:74:A:SER:N	1:74:A:SER:CA	1:74:A:SER:C	18	1.86
(1,179)	1:125:A:VAL:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	6	1.85
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	6	1.84
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	17	1.84
(1,179)	1:125:A:VAL:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	18	1.83
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	14	1.82
(1,98)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:LEU:N	9	1.8
(1,165)	1:118:A:SER:C	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	19	1.79
(1,127)	1:94:A:LEU:C	1:95:A:PHE:N	1:95:A:PHE:CA	1:95:A:PHE:C	17	1.78
(1,123)	1:92:A:ASN:C	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	13	1.77
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	12	1.76
(1,115)	1:88:A:GLU:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	19	1.76
(1,178)	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	1:126:A:LEU:N	6	1.75
(1,229)	1:155:A:PHE:C	1:156:A:VAL:N	1:156:A:VAL:CA	1:156:A:VAL:C	7	1.74
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	11	1.73
(1,207)	1:139:A:ASN:C	1:140:A:ASP:N	1:140:A:ASP:CA	1:140:A:ASP:C	13	1.73
(1,247)	1:176:A:HIS:C	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	17	1.7
(1,219)	1:148:A:GLU:C	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	10	1.69
(1,108)	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	1:85:A:GLN:N	7	1.67
(1,90)	1:67:A:ARG:N	1:67:A:ARG:CA	1:67:A:ARG:C	1:68:A:ALA:N	17	1.65
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	19	1.64
(1,19)	1:12:A:LEU:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	19	1.63
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	7	1.61
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	15	1.6
(1,134)	1:102:A:GLY:N	1:102:A:GLY:CA	1:102:A:GLY:C	1:103:A:ARG:N	8	1.59
(1,235)	1:162:A:ASN:C	1:163:A:ALA:N	1:163:A:ALA:CA	1:163:A:ALA:C	18	1.58
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	4	1.58
(1,217)	1:147:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	16	1.58
(1,101)	1:72:A:LEU:C	1:73:A:THR:N	1:73:A:THR:CA	1:73:A:THR:C	9	1.58
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	8	1.57
(1,114)	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	1:89:A:GLN:N	10	1.56
(1,98)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:LEU:N	4	1.55
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	6	1.5
(1,218)	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1:149:A:ASN:N	18	1.47
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	8	1.47
(1,51)	1:31:A:PHE:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	8	1.47
(1,221)	1:151:A:GLY:C	1:152:A:TRP:N	1:152:A:TRP:CA	1:152:A:TRP:C	9	1.46
(1,165)	1:118:A:SER:C	1:119:A:VAL:N	1:119:A:VAL:CA	1:119:A:VAL:C	11	1.46
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	2	1.44
(1,123)	1:92:A:ASN:C	1:93:A:GLU:N	1:93:A:GLU:CA	1:93:A:GLU:C	16	1.43
(1,98)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:LEU:N	12	1.43
(1,66)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:LEU:N	16	1.43
(1,71)	1:55:A:ARG:C	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	13	1.4
(1,159)	1:115:A:CYS:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	5	1.38
(1,44)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:TRP:N	19	1.38
(1,15)	1:10:A:ARG:C	1:11:A:GLU:N	1:11:A:GLU:CA	1:11:A:GLU:C	8	1.38
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	19	1.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,220)	1:149:A:ASN:N	1:149:A:ASN:CA	1:149:A:ASN:C	1:150:A:GLY:N	20	1.34
(1,175)	1:123:A:MET:C	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	11	1.34
(1,229)	1:155:A:PHE:C	1:156:A:VAL:N	1:156:A:VAL:CA	1:156:A:VAL:C	16	1.33
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	7	1.33
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:SER:N	5	1.32
(1,201)	1:136:A:THR:C	1:137:A:TYR:N	1:137:A:TYR:CA	1:137:A:TYR:C	16	1.31
(1,129)	1:95:A:PHE:C	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	17	1.29
(1,107)	1:83:A:ALA:C	1:84:A:TYR:N	1:84:A:TYR:CA	1:84:A:TYR:C	18	1.28
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	10	1.27
(1,120)	1:91:A:VAL:N	1:91:A:VAL:CA	1:91:A:VAL:C	1:92:A:ASN:N	13	1.27
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	9	1.26
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	17	1.25
(1,98)	1:71:A:ASP:N	1:71:A:ASP:CA	1:71:A:ASP:C	1:72:A:LEU:N	10	1.23
(1,67)	1:53:A:ALA:C	1:54:A:LEU:N	1:54:A:LEU:CA	1:54:A:LEU:C	3	1.23
(1,167)	1:119:A:VAL:C	1:120:A:ASP:N	1:120:A:ASP:CA	1:120:A:ASP:C	20	1.19
(1,137)	1:103:A:ARG:C	1:104:A:ILE:N	1:104:A:ILE:CA	1:104:A:ILE:C	2	1.19
(1,214)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:GLN:N	20	1.18
(1,183)	1:127:A:VAL:C	1:128:A:SER:N	1:128:A:SER:CA	1:128:A:SER:C	16	1.18
(1,21)	1:13:A:VAL:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	16	1.14
(1,202)	1:137:A:TYR:N	1:137:A:TYR:CA	1:137:A:TYR:C	1:138:A:LEU:N	16	1.12
(1,186)	1:129:A:ARG:N	1:129:A:ARG:CA	1:129:A:ARG:C	1:130:A:ILE:N	19	1.12
(1,62)	1:51:A:LYS:N	1:51:A:LYS:CA	1:51:A:LYS:C	1:52:A:GLN:N	17	1.11
(1,22)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:ASP:N	12	1.11
(1,189)	1:130:A:ILE:C	1:131:A:ALA:N	1:131:A:ALA:CA	1:131:A:ALA:C	7	1.09
(1,23)	1:14:A:VAL:C	1:15:A:ASP:N	1:15:A:ASP:CA	1:15:A:ASP:C	6	1.09
(1,217)	1:147:A:GLN:C	1:148:A:GLU:N	1:148:A:GLU:CA	1:148:A:GLU:C	1	1.06
(1,9)	1:7:A:GLN:C	1:8:A:SER:N	1:8:A:SER:CA	1:8:A:SER:C	15	1.04
(1,229)	1:155:A:PHE:C	1:156:A:VAL:N	1:156:A:VAL:CA	1:156:A:VAL:C	2	1.03
(1,175)	1:123:A:MET:C	1:124:A:GLN:N	1:124:A:GLN:CA	1:124:A:GLN:C	17	1.01
(1,206)	1:139:A:ASN:N	1:139:A:ASN:CA	1:139:A:ASN:C	1:140:A:ASP:N	19	1.0