Full wwPDB NMR Structure Validation Report (i)

Mar 4, 2026 – 09:21 PM UTC

PDB ID	:	2KMT / pdb_00002kmt
BMRB ID	:	16135
Title	:	NMR solution structure of Vibrio fischeri CcdB
Authors	:	Zangger, K.
Deposited on	:	2009-08-04

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

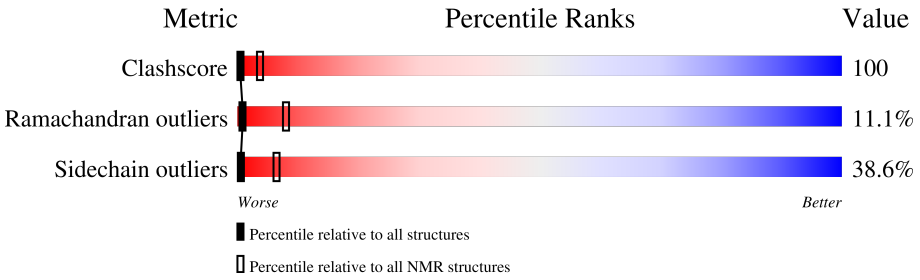
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 41%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	105	19% 46% 32%
1	B	105	18% 49% 31%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:2-A:105, B:1-B:105 (209)	1.00	8

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3386 atoms, of which 1718 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CcdB.

Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1693	538	859	131	161	4	
1	B	105	Total	C	H	N	O	S	0
			1693	538	859	131	161	4	

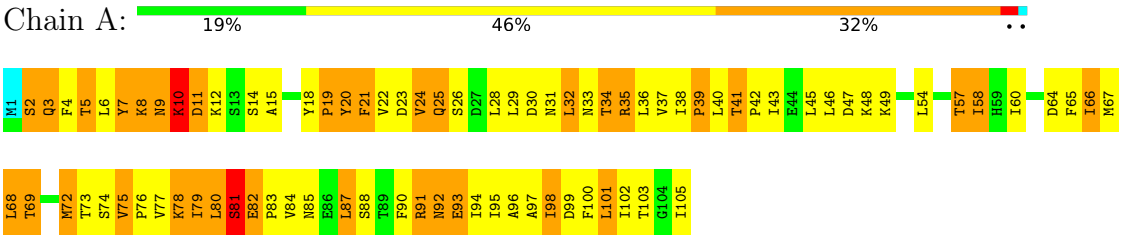
4 Residue-property plots

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.

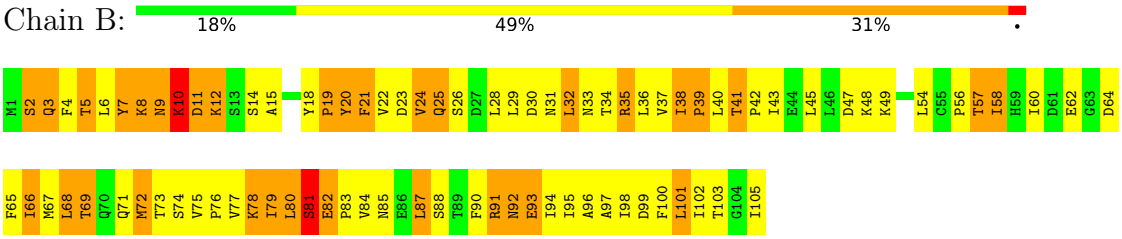
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

Chain B:



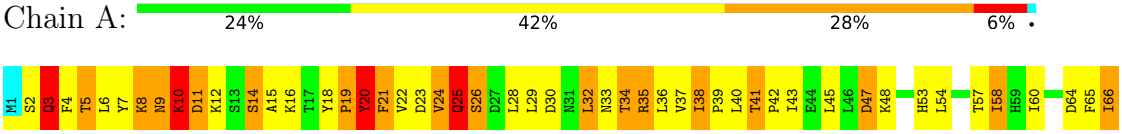
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

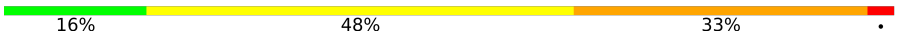
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

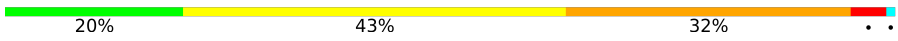
Chain B:

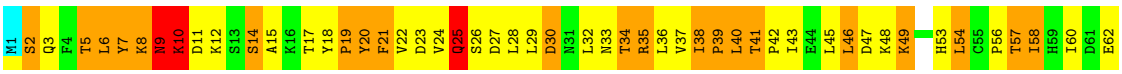


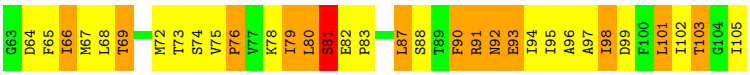
4.2.2 Score per residue for model 2

• Molecule 1: CcdB

Chain A:

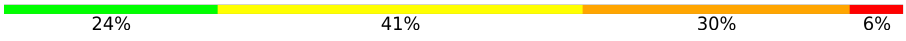


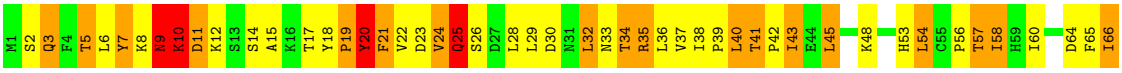


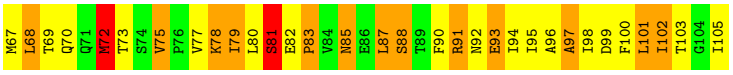


• Molecule 1: CcdB

Chain B:



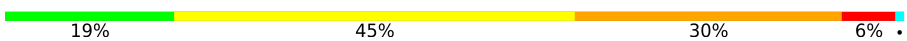


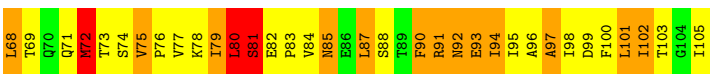


4.2.3 Score per residue for model 3

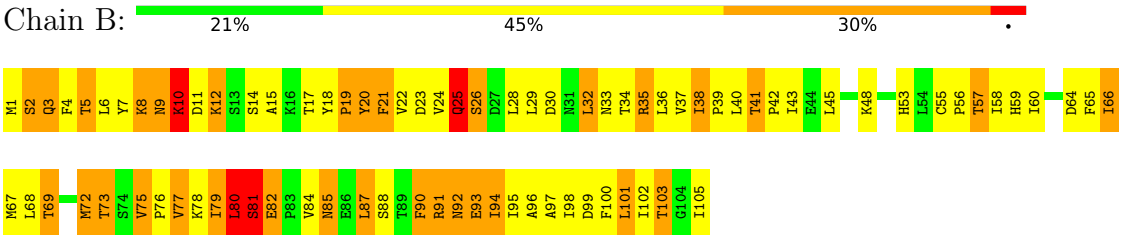
• Molecule 1: CcdB

Chain A:



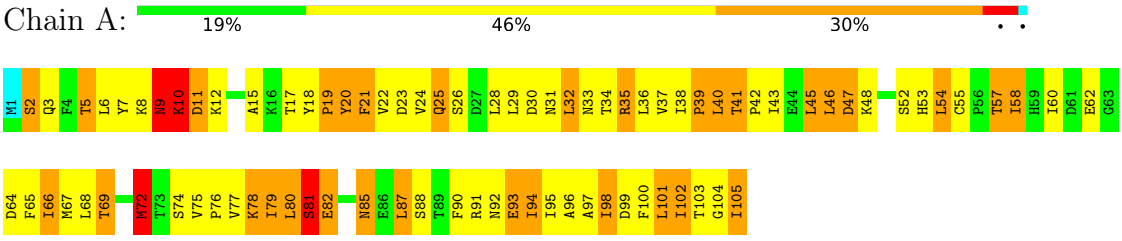


• Molecule 1: CcdB

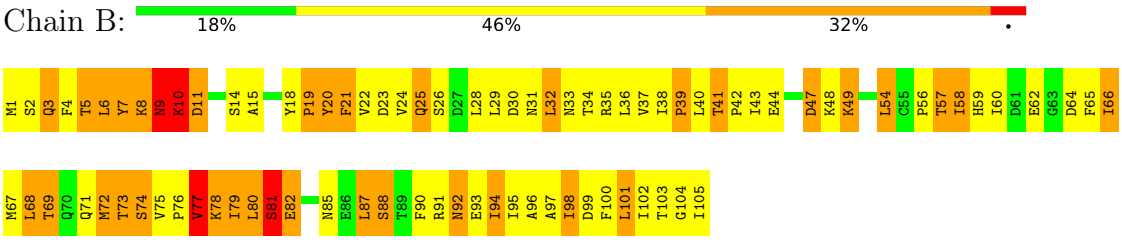


4.2.4 Score per residue for model 4

- Molecule 1: CcdB

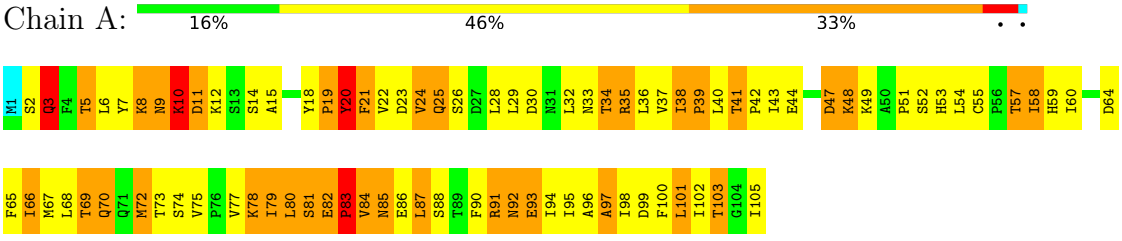


- Molecule 1: CcdB

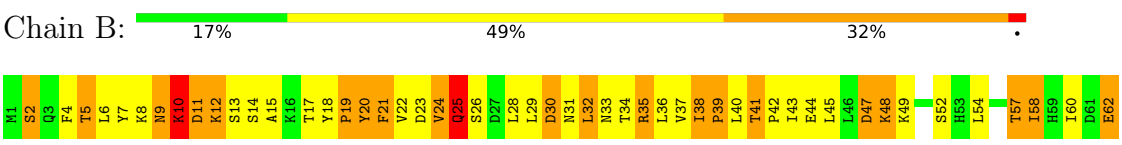


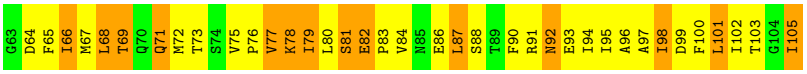
4.2.5 Score per residue for model 5

- Molecule 1: CcdB



- Molecule 1: CcdB

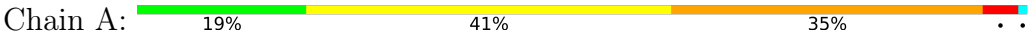




4.2.6 Score per residue for model 6

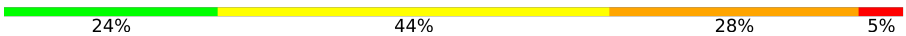
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

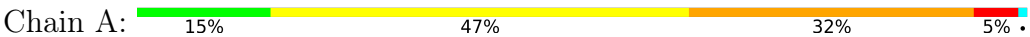
Chain B:

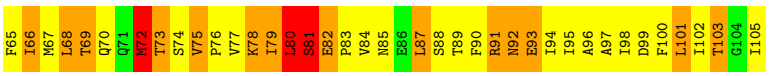


4.2.7 Score per residue for model 7

• Molecule 1: CcdB

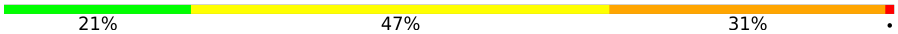
Chain A:

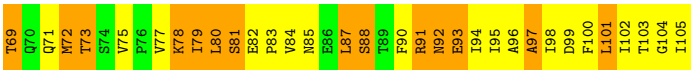




• Molecule 1: CcdB

Chain B:

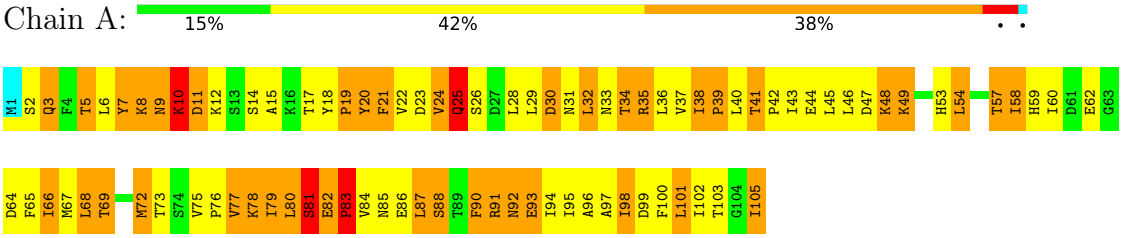




4.2.8 Score per residue for model 8 (medoid)

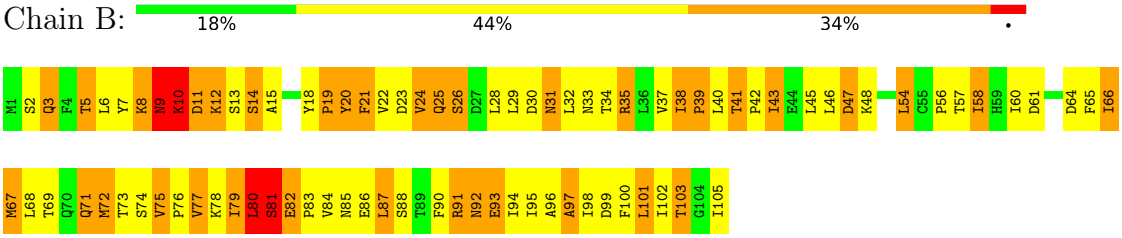
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

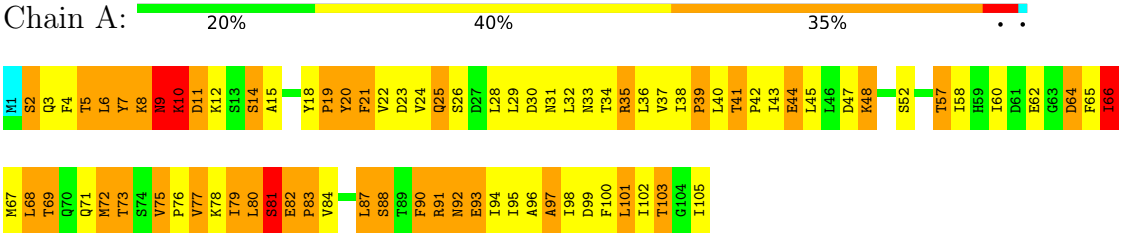
Chain B:



4.2.9 Score per residue for model 9

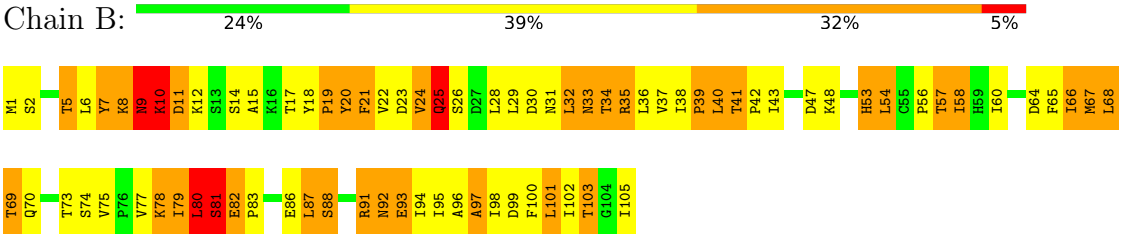
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

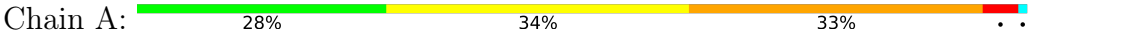
Chain B:

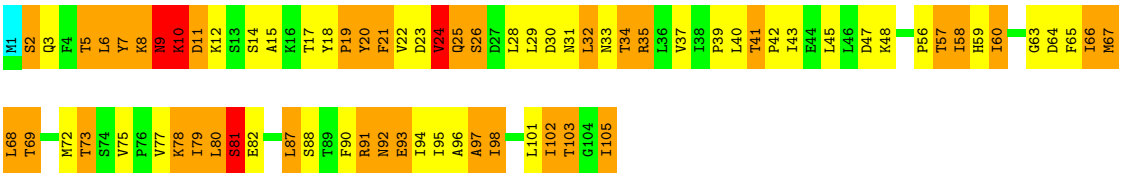


4.2.10 Score per residue for model 10

• Molecule 1: CcdB

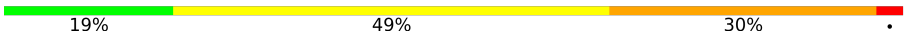
Chain A:

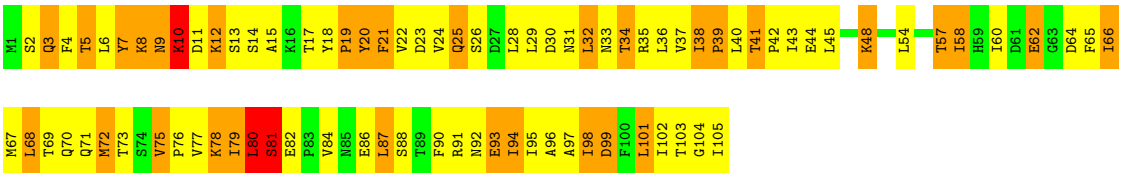




• Molecule 1: CcdB

Chain B:





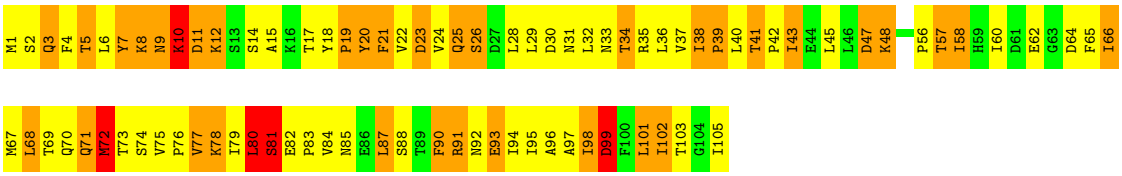
4.2.11 Score per residue for model 11

• Molecule 1: CcdB

Chain A:

• Molecule 1: CcdB

Chain B:



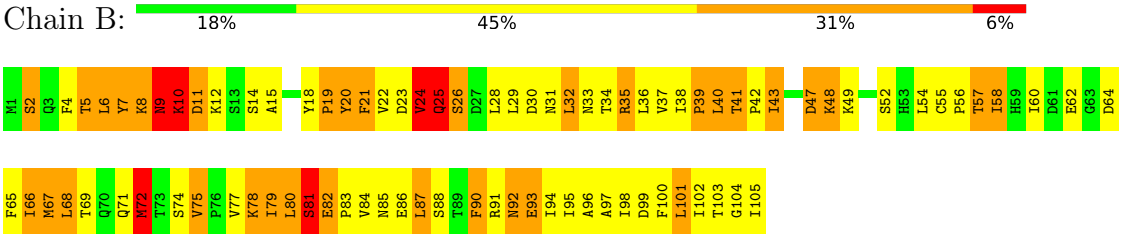
4.2.12 Score per residue for model 12

• Molecule 1: CcdB

Chain A:

• Molecule 1: CcdB

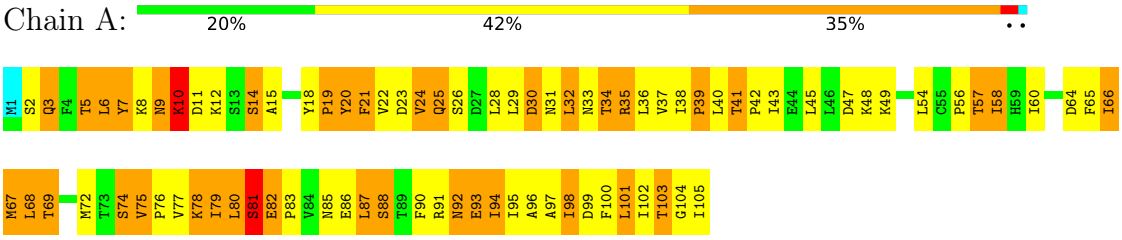
Chain B:



4.2.13 Score per residue for model 13

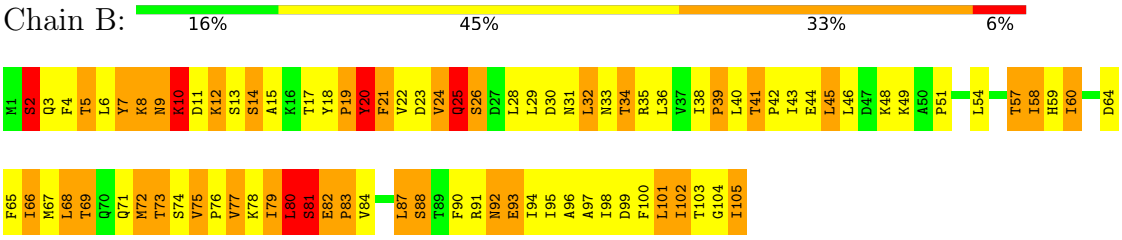
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

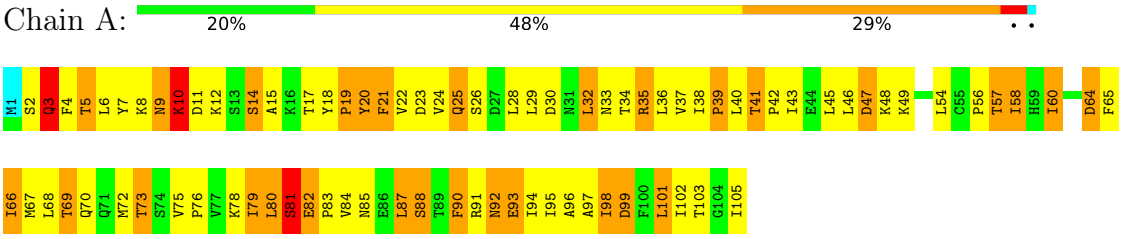
Chain B:



4.2.14 Score per residue for model 14

• Molecule 1: CcdB

Chain A:



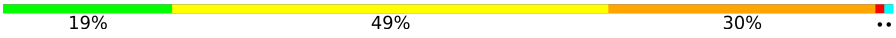
• Molecule 1: CcdB

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

Chain B:

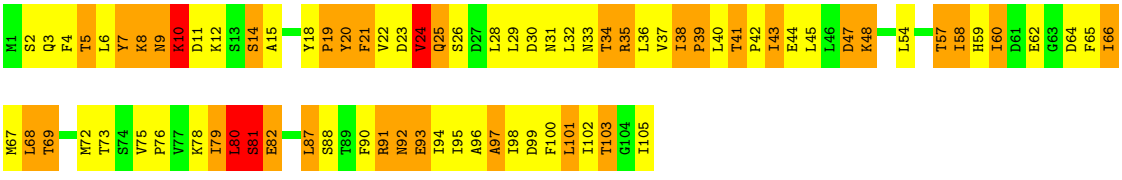
4.2.16 Score per residue for model 16

• Molecule 1: CcdB

Chain A:

• Molecule 1: CcdB

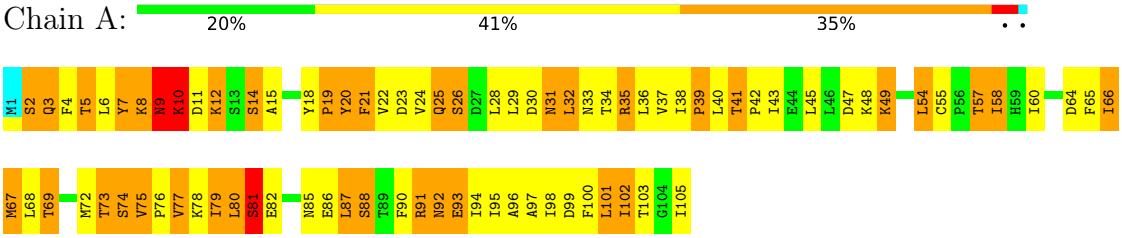
Chain B:



4.2.17 Score per residue for model 17

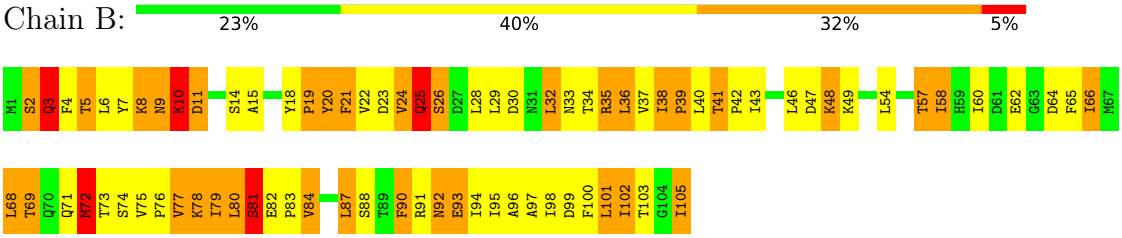
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

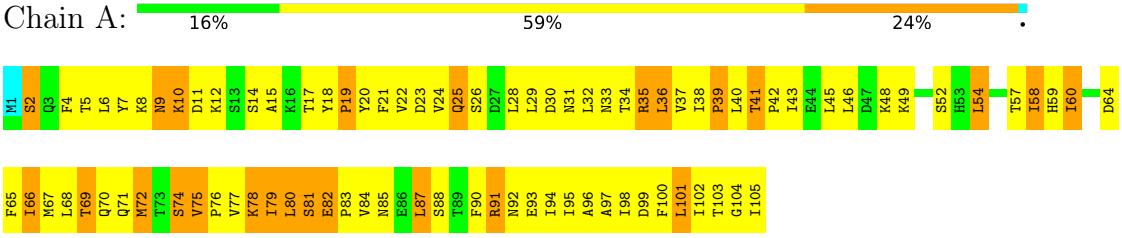
Chain B:



4.2.18 Score per residue for model 18

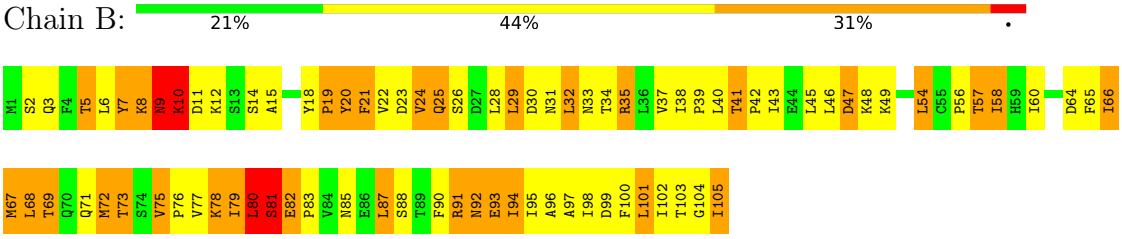
• Molecule 1: CcdB

Chain A:



• Molecule 1: CcdB

Chain B:

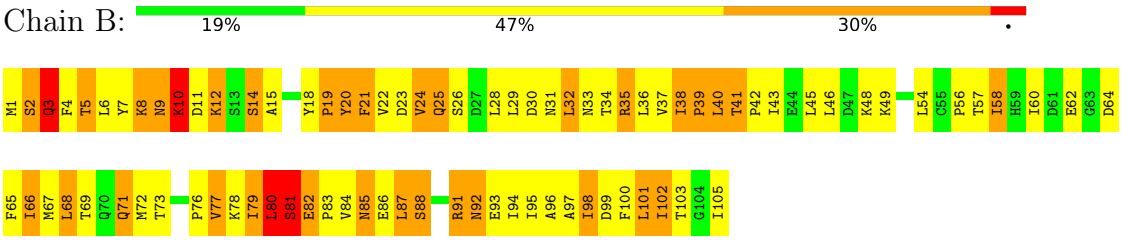


4.2.19 Score per residue for model 19

• Molecule 1: CcdB

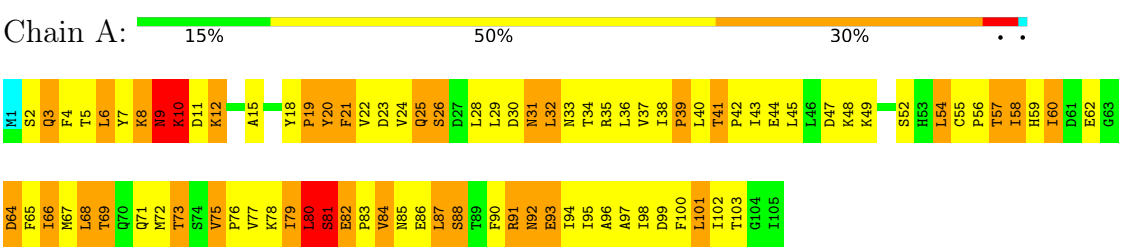
Chain A:

• Molecule 1: CcdB

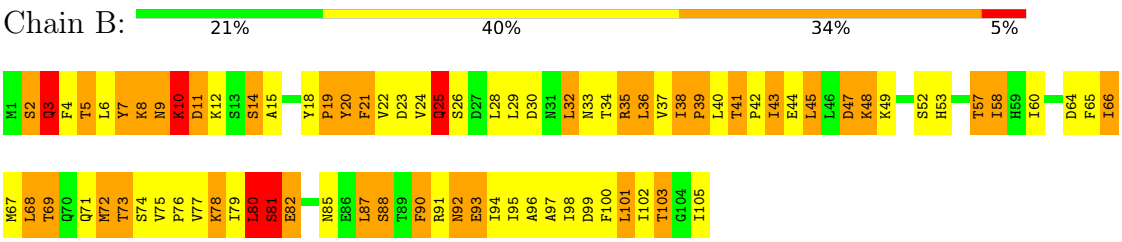


4.2.20 Score per residue for model 20

• Molecule 1: CcdB



• Molecule 1: CcdB



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CNS	structure solution	
CNS	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	1186
Number of shifts mapped to atoms	1186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.52±0.01	0±0/842 (0.0± 0.0%)	0.86±0.02	0±0/1145 (0.0± 0.0%)
1	B	0.53±0.01	0±0/850 (0.0± 0.0%)	0.86±0.02	0±1/1155 (0.0± 0.0%)
All	All	0.53	0/33840 (0.0%)	0.86	12/46000 (0.0%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	20	TYR	N-CA-C	7.18	118.08	108.38	15	4
1	A	20	TYR	N-CA-C	5.48	116.30	108.74	7	7
1	B	41	THR	N-CA-C	5.44	113.11	108.22	15	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	826	848	846	167±11
1	B	834	859	857	174±12
All	All	33200	34140	34060	6716

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 100.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ILE:HD12	1:B:69:THR:HG23	1.14	1.20	9	3
1:B:8:LYS:HA	1:B:20:TYR:HB3	1.06	1.25	15	18
1:A:58:ILE:HD13	1:A:60:ILE:HG23	1.05	1.19	10	2
1:B:58:ILE:HD13	1:B:60:ILE:HG23	1.05	1.09	1	1
1:B:72:MET:HE1	1:B:101:LEU:HD21	1.01	1.27	19	3
1:B:30:ASP:O	1:B:35:ARG:HB2	1.00	1.57	20	8
1:B:69:THR:HG22	1:B:101:LEU:HD22	1.00	1.33	20	6
1:B:29:LEU:HD23	1:B:32:LEU:HD22	1.00	1.30	6	5
1:B:40:LEU:HD21	1:B:67:MET:HE2	1.00	1.24	8	1
1:B:54:LEU:HD23	1:B:69:THR:HG23	0.99	1.27	8	2
1:A:40:LEU:HD21	1:A:67:MET:HE3	0.99	1.29	13	1
1:A:69:THR:HG22	1:A:101:LEU:HD22	0.97	1.34	4	7
1:A:29:LEU:HD23	1:A:32:LEU:HD22	0.97	1.30	17	7
1:A:22:VAL:HG11	1:A:94:ILE:CG1	0.97	1.89	8	17
1:A:40:LEU:HD21	1:A:67:MET:HE2	0.96	1.35	6	1
1:A:24:VAL:HG21	1:A:98:ILE:HD11	0.95	1.39	18	1
1:B:43:ILE:HD11	1:B:57:THR:OG1	0.94	1.62	5	10
1:B:22:VAL:HG11	1:B:94:ILE:CG1	0.94	1.92	19	15
1:A:60:ILE:HD11	1:A:87:LEU:HD23	0.94	1.36	15	1
1:B:41:THR:HG23	1:B:66:ILE:CD1	0.93	1.94	15	15
1:A:43:ILE:HD11	1:A:57:THR:OG1	0.92	1.63	10	12
1:A:58:ILE:HD12	1:A:59:HIS:N	0.92	1.80	19	2
1:A:58:ILE:HG23	1:A:90:PHE:CE2	0.91	1.99	4	8
1:A:29:LEU:HD23	1:A:32:LEU:HD12	0.91	1.42	18	5
1:A:41:THR:HG23	1:A:66:ILE:CD1	0.91	1.96	5	18
1:B:101:LEU:C	1:B:101:LEU:HD22	0.91	1.91	13	3
1:A:58:ILE:HG21	1:A:87:LEU:HD12	0.90	1.42	14	7
1:B:36:LEU:HD11	1:B:72:MET:HE3	0.90	1.42	14	1
1:B:58:ILE:HG21	1:B:87:LEU:HD12	0.90	1.41	7	4
1:A:101:LEU:HD22	1:A:101:LEU:C	0.89	1.91	15	1
1:A:6:LEU:HD11	1:A:60:ILE:HD13	0.89	1.44	12	8
1:A:6:LEU:HD21	1:A:60:ILE:HD13	0.88	1.43	17	2
1:A:36:LEU:HD21	1:A:72:MET:HE3	0.88	1.43	16	4
1:B:10:LYS:N	1:B:81:SER:HA	0.86	1.86	3	20
1:A:10:LYS:N	1:A:81:SER:HA	0.86	1.84	14	19
1:B:29:LEU:HD23	1:B:32:LEU:HD12	0.86	1.47	18	5
1:A:79:ILE:HG12	1:A:79:ILE:O	0.86	1.68	18	8
1:B:22:VAL:HG21	1:B:67:MET:HE3	0.86	1.46	6	7
1:A:58:ILE:CD1	1:A:60:ILE:HG23	0.86	2.00	19	2
1:B:36:LEU:HD21	1:B:72:MET:HE3	0.85	1.45	16	2
1:B:54:LEU:CD2	1:B:69:THR:HG23	0.85	1.99	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:22:VAL:CG1	1:B:94:ILE:HD13	0.85	2.00	1	3
1:A:40:LEU:HD21	1:A:67:MET:CE	0.85	2.02	13	2
1:A:45:LEU:O	1:A:45:LEU:HD12	0.85	1.72	4	1
1:B:58:ILE:HG23	1:B:90:PHE:CE2	0.85	2.07	18	9
1:A:8:LYS:HA	1:A:20:TYR:HB3	0.85	1.47	16	17
1:B:45:LEU:HD12	1:B:45:LEU:O	0.85	1.72	13	2
1:B:29:LEU:HD23	1:B:32:LEU:CD1	0.85	2.02	18	7
1:B:101:LEU:HD13	1:B:102:ILE:HG13	0.84	1.49	13	3
1:B:72:MET:HE1	1:B:98:ILE:HD11	0.84	1.49	12	1
1:B:36:LEU:HD13	1:B:37:VAL:N	0.84	1.88	7	2
1:B:58:ILE:HG21	1:B:87:LEU:HD23	0.84	1.48	18	7
1:B:22:VAL:HG11	1:B:94:ILE:HG13	0.84	1.50	12	15
1:A:54:LEU:HD23	1:A:69:THR:HG23	0.83	1.48	3	1
1:A:58:ILE:HD12	1:A:58:ILE:C	0.83	1.98	19	2
1:A:22:VAL:HG11	1:A:94:ILE:HG12	0.83	1.50	5	16
1:A:29:LEU:HD23	1:A:32:LEU:CD1	0.83	2.03	15	5
1:A:38:ILE:HD12	1:A:69:THR:HG23	0.83	1.50	18	2
1:B:58:ILE:HD11	1:B:65:PHE:HB2	0.82	1.50	8	7
1:A:8:LYS:O	1:A:20:TYR:HA	0.82	1.74	15	6
1:A:57:THR:OG1	1:A:66:ILE:HG23	0.82	1.74	13	13
1:B:75:VAL:HG23	1:B:79:ILE:HD13	0.82	1.49	3	7
1:A:22:VAL:HG11	1:A:94:ILE:HD13	0.82	1.50	3	5
1:A:5:THR:HB	1:A:7:TYR:CE1	0.82	2.09	20	20
1:B:58:ILE:HD12	1:B:87:LEU:HD22	0.82	1.51	18	4
1:B:38:ILE:CG2	1:B:67:MET:HE2	0.82	2.04	2	1
1:B:8:LYS:O	1:B:20:TYR:HA	0.82	1.73	13	2
1:A:72:MET:HE1	1:A:101:LEU:HD21	0.82	1.47	6	2
1:A:43:ILE:HD11	1:A:57:THR:CG2	0.81	2.05	19	1
1:B:58:ILE:C	1:B:58:ILE:HD12	0.81	2.00	1	1
1:A:25:GLN:OE1	1:B:101:LEU:HD12	0.81	1.75	8	3
1:A:30:ASP:O	1:A:35:ARG:HB2	0.81	1.75	2	5
1:A:75:VAL:HG23	1:A:79:ILE:HD13	0.81	1.53	6	5
1:A:58:ILE:HG21	1:A:87:LEU:HD23	0.81	1.52	17	4
1:A:10:LYS:HG2	1:A:79:ILE:HG22	0.81	1.52	13	1
1:B:102:ILE:HD12	1:B:103:THR:HG23	0.81	1.52	19	1
1:B:8:LYS:O	1:B:82:GLU:N	0.81	2.14	17	18
1:A:6:LEU:HD12	1:A:84:VAL:HG23	0.81	1.51	20	1
1:A:58:ILE:HA	1:A:90:PHE:CZ	0.80	2.11	8	14
1:B:58:ILE:CG2	1:B:60:ILE:HG23	0.80	2.06	16	5
1:A:7:TYR:C	1:A:81:SER:HB3	0.80	2.01	6	5
1:B:10:LYS:HG2	1:B:79:ILE:HG22	0.80	1.53	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD12	1:B:25:GLN:OE1	0.80	1.77	1	1
1:A:22:VAL:HG11	1:A:94:ILE:HG13	0.80	1.53	8	12
1:A:58:ILE:CG2	1:A:60:ILE:HG23	0.80	2.06	18	5
1:A:60:ILE:HD11	1:A:87:LEU:CD2	0.80	2.07	15	1
1:B:6:LEU:HD21	1:B:60:ILE:HD13	0.80	1.53	19	4
1:A:101:LEU:HD13	1:A:102:ILE:HG13	0.80	1.51	15	1
1:A:35:ARG:HA	1:A:35:ARG:NE	0.79	1.92	3	2
1:A:22:VAL:HG11	1:A:94:ILE:CD1	0.79	2.06	10	6
1:A:8:LYS:O	1:A:82:GLU:N	0.79	2.14	9	12
1:B:22:VAL:HG11	1:B:94:ILE:HG12	0.79	1.54	9	15
1:B:25:GLN:NE2	1:B:36:LEU:HD22	0.79	1.91	14	1
1:B:31:ASN:OD1	1:B:80:LEU:HD12	0.79	1.78	14	2
1:A:30:ASP:O	1:A:35:ARG:HB3	0.79	1.76	8	7
1:A:43:ILE:HD12	1:A:57:THR:OG1	0.79	1.78	6	4
1:B:22:VAL:HG11	1:B:94:ILE:HD13	0.79	1.52	10	3
1:B:57:THR:OG1	1:B:66:ILE:HG23	0.79	1.75	13	14
1:A:22:VAL:CG1	1:A:94:ILE:HD13	0.79	2.08	3	5
1:B:29:LEU:CD2	1:B:32:LEU:HD22	0.79	2.08	7	3
1:A:102:ILE:HG21	1:B:102:ILE:HD13	0.79	1.52	9	3
1:A:35:ARG:CZ	1:A:80:LEU:HD22	0.78	2.08	6	4
1:B:99:ASP:CG	1:B:105:ILE:HD11	0.78	2.03	9	4
1:B:5:THR:HB	1:B:7:TYR:CE1	0.78	2.14	5	20
1:B:101:LEU:C	1:B:101:LEU:CD2	0.78	2.56	6	3
1:B:23:ASP:OD1	1:B:80:LEU:HD11	0.78	1.79	9	8
1:B:58:ILE:HA	1:B:90:PHE:CZ	0.78	2.14	11	15
1:B:58:ILE:HG23	1:B:90:PHE:CD2	0.78	2.14	14	8
1:B:36:LEU:HD21	1:B:72:MET:CE	0.78	2.08	4	3
1:A:58:ILE:HD11	1:A:65:PHE:HB2	0.78	1.55	13	8
1:B:38:ILE:HG21	1:B:69:THR:HG23	0.78	1.54	1	10
1:B:7:TYR:C	1:B:81:SER:HB3	0.78	2.04	16	7
1:B:22:VAL:C	1:B:37:VAL:HG12	0.78	2.03	5	13
1:A:43:ILE:HD11	1:A:57:THR:HB	0.78	1.56	18	2
1:B:57:THR:HA	1:B:65:PHE:O	0.77	1.79	3	14
1:A:10:LYS:N	1:A:10:LYS:CD	0.77	2.47	20	15
1:B:24:VAL:HG22	1:B:98:ILE:HD12	0.77	1.56	5	4
1:A:99:ASP:CG	1:A:105:ILE:HD11	0.77	2.04	5	2
1:A:22:VAL:C	1:A:37:VAL:HG12	0.77	2.04	4	15
1:A:67:MET:HE1	1:A:94:ILE:HG13	0.77	1.56	2	1
1:B:43:ILE:HD11	1:B:57:THR:HG23	0.77	1.54	1	1
1:B:38:ILE:CD1	1:B:69:THR:HG23	0.77	2.06	9	2
1:B:41:THR:HG23	1:B:66:ILE:HD13	0.77	1.55	4	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:ILE:HD13	1:B:60:ILE:CG2	0.77	2.03	1	1
1:B:23:ASP:OD2	1:B:80:LEU:HD21	0.77	1.80	2	1
1:A:101:LEU:C	1:A:101:LEU:CD2	0.76	2.57	15	1
1:A:29:LEU:HD23	1:A:32:LEU:HD13	0.76	1.55	7	4
1:A:58:ILE:HG22	1:A:60:ILE:HG23	0.76	1.57	8	7
1:A:6:LEU:HD11	1:A:20:TYR:CD2	0.76	2.14	4	1
1:A:102:ILE:CD1	1:A:103:THR:HG23	0.76	2.11	6	4
1:A:40:LEU:CD2	1:A:67:MET:HE2	0.76	2.10	6	1
1:B:20:TYR:CE1	1:B:40:LEU:HB2	0.76	2.15	15	1
1:A:41:THR:HG23	1:A:66:ILE:HD13	0.76	1.56	9	16
1:B:35:ARG:NE	1:B:35:ARG:HA	0.76	1.95	18	4
1:B:4:PHE:CD1	1:B:94:ILE:HD12	0.76	2.15	10	2
1:A:58:ILE:HG23	1:A:90:PHE:CD2	0.76	2.16	4	7
1:A:38:ILE:HG21	1:A:69:THR:HG23	0.76	1.58	11	9
1:A:7:TYR:C	1:A:81:SER:HB2	0.76	2.05	2	11
1:A:10:LYS:N	1:A:10:LYS:HD2	0.76	1.95	18	7
1:A:72:MET:HE1	1:A:101:LEU:CD2	0.76	2.10	6	1
1:B:9:ASN:OD1	1:B:19:PRO:HA	0.76	1.81	14	4
1:B:6:LEU:CD1	1:B:60:ILE:HG21	0.75	2.11	5	6
1:B:6:LEU:HD12	1:B:60:ILE:HG21	0.75	1.58	7	4
1:B:22:VAL:O	1:B:24:VAL:HG13	0.75	1.80	17	2
1:A:9:ASN:OD1	1:A:11:ASP:O	0.75	2.04	19	1
1:A:10:LYS:CD	1:A:10:LYS:N	0.75	2.50	7	2
1:A:56:PRO:O	1:A:67:MET:HE3	0.75	1.80	6	1
1:A:67:MET:HE1	1:A:94:ILE:HD12	0.75	1.57	12	2
1:B:10:LYS:N	1:B:10:LYS:CD	0.75	2.48	13	20
1:B:8:LYS:C	1:B:19:PRO:O	0.75	2.30	1	2
1:A:91:ARG:HA	1:A:94:ILE:HD12	0.75	1.56	2	4
1:A:8:LYS:C	1:A:19:PRO:O	0.75	2.29	8	6
1:A:24:VAL:CG1	1:A:94:ILE:HG23	0.75	2.11	18	1
1:B:24:VAL:HG11	1:B:38:ILE:HD11	0.75	1.59	20	3
1:B:6:LEU:HD11	1:B:60:ILE:HD13	0.74	1.57	5	4
1:A:89:THR:HG23	1:A:90:PHE:CD1	0.74	2.16	7	1
1:B:10:LYS:HG2	1:B:79:ILE:CD1	0.74	2.11	7	1
1:A:73:THR:OG1	1:B:73:THR:HG22	0.74	1.82	14	3
1:B:20:TYR:OH	1:B:65:PHE:CE1	0.74	2.39	4	15
1:B:38:ILE:CG2	1:B:69:THR:HG23	0.74	2.13	13	12
1:A:73:THR:CB	1:B:73:THR:HG22	0.74	2.12	11	2
1:B:58:ILE:HD13	1:B:90:PHE:CE2	0.74	2.18	17	2
1:A:10:LYS:HB3	1:A:79:ILE:HG12	0.74	1.58	18	1
1:A:38:ILE:HB	1:A:67:MET:HE2	0.74	1.60	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:30:ASP:O	1:B:35:ARG:HB3	0.74	1.83	17	4
1:B:102:ILE:CD1	1:B:103:THR:HG23	0.74	2.12	10	3
1:A:6:LEU:CD1	1:A:60:ILE:HD13	0.74	2.13	3	6
1:A:69:THR:OG1	1:A:101:LEU:HD22	0.74	1.82	3	3
1:B:29:LEU:HD23	1:B:32:LEU:HD13	0.74	1.56	17	6
1:B:42:PRO:HA	1:B:65:PHE:CD1	0.74	2.17	15	1
1:B:43:ILE:HG23	1:B:48:LYS:HG2	0.74	1.60	17	1
1:B:10:LYS:HD3	1:B:10:LYS:N	0.74	1.98	11	5
1:A:73:THR:HB	1:B:73:THR:HG22	0.74	1.60	11	2
1:B:58:ILE:HD13	1:B:90:PHE:CD2	0.74	2.17	20	3
1:A:35:ARG:NH1	1:A:80:LEU:HD22	0.74	1.96	6	3
1:B:36:LEU:HD11	1:B:72:MET:HG2	0.73	1.59	11	4
1:B:56:PRO:O	1:B:67:MET:HE3	0.73	1.82	8	2
1:B:79:ILE:HG12	1:B:79:ILE:O	0.73	1.82	17	7
1:B:10:LYS:N	1:B:10:LYS:HD2	0.73	1.99	8	5
1:A:8:LYS:CE	1:A:15:ALA:HB2	0.73	2.13	18	1
1:B:33:ASN:O	1:B:34:THR:HG23	0.73	1.82	19	8
1:A:35:ARG:NH1	1:A:80:LEU:HD11	0.73	1.98	16	1
1:B:29:LEU:HD23	1:B:32:LEU:CD2	0.73	2.10	6	2
1:A:22:VAL:HG21	1:A:67:MET:CE	0.73	2.12	17	1
1:A:38:ILE:CG2	1:A:69:THR:HG23	0.73	2.13	5	11
1:B:69:THR:HG22	1:B:101:LEU:HD12	0.73	1.60	6	2
1:A:35:ARG:CZ	1:A:75:VAL:HB	0.73	2.13	18	1
1:A:99:ASP:O	1:A:103:THR:HG23	0.73	1.83	20	1
1:B:7:TYR:CD2	1:B:80:LEU:HD12	0.73	2.18	18	5
1:A:69:THR:HG21	1:A:97:ALA:HB1	0.73	1.58	13	4
1:B:58:ILE:HD12	1:B:87:LEU:CD2	0.73	2.14	20	4
1:A:72:MET:HE3	1:A:102:ILE:HD11	0.73	1.58	19	2
1:A:20:TYR:OH	1:A:65:PHE:CE1	0.73	2.41	15	18
1:B:76:PRO:O	1:B:79:ILE:HD12	0.73	1.83	15	10
1:B:69:THR:OG1	1:B:101:LEU:HD22	0.72	1.84	8	3
1:B:6:LEU:HD12	1:B:87:LEU:HD13	0.72	1.60	13	1
1:B:24:VAL:CG1	1:B:94:ILE:HG23	0.72	2.14	15	1
1:B:24:VAL:HG21	1:B:38:ILE:CD1	0.72	2.14	15	1
1:B:24:VAL:HG21	1:B:98:ILE:HD11	0.72	1.61	17	2
1:B:10:LYS:HD2	1:B:10:LYS:N	0.72	2.00	19	2
1:B:67:MET:HE1	1:B:94:ILE:HG13	0.72	1.58	7	6
1:B:7:TYR:C	1:B:81:SER:HB2	0.72	2.09	7	12
1:A:75:VAL:HG12	1:A:79:ILE:HD13	0.72	1.58	15	4
1:B:72:MET:SD	1:B:101:LEU:HD11	0.72	2.24	14	2
1:B:75:VAL:HG12	1:B:79:ILE:HD13	0.72	1.59	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:CD2	1:A:72:MET:HE3	0.72	2.15	16	1
1:B:8:LYS:HE3	1:B:15:ALA:HB2	0.72	1.61	2	1
1:B:4:PHE:CZ	1:B:95:ILE:HD11	0.72	2.20	5	6
1:B:24:VAL:HG11	1:B:38:ILE:CD1	0.72	2.15	17	5
1:A:6:LEU:HD13	1:A:60:ILE:HD13	0.72	1.62	18	3
1:B:40:LEU:HD23	1:B:67:MET:HG2	0.72	1.61	15	4
1:B:8:LYS:C	1:B:81:SER:HB3	0.71	2.10	1	4
1:A:24:VAL:HG11	1:A:38:ILE:HD11	0.71	1.61	8	6
1:A:58:ILE:HD13	1:A:90:PHE:CD2	0.71	2.20	3	3
1:A:25:GLN:NE2	1:B:101:LEU:HD11	0.71	1.99	18	5
1:A:6:LEU:CD1	1:A:60:ILE:HG21	0.71	2.15	18	2
1:A:22:VAL:O	1:A:37:VAL:HG12	0.71	1.85	1	6
1:B:10:LYS:HB3	1:B:79:ILE:HB	0.71	1.61	15	4
1:B:21:PHE:CD2	1:B:75:VAL:HG21	0.71	2.19	18	1
1:B:56:PRO:HD2	1:B:67:MET:HB2	0.71	1.62	12	4
1:A:33:ASN:O	1:A:34:THR:HG23	0.71	1.85	18	8
1:A:29:LEU:HD23	1:A:32:LEU:CD2	0.71	2.13	17	3
1:A:67:MET:HE2	1:A:94:ILE:HG13	0.71	1.61	10	1
1:A:101:LEU:HD11	1:B:25:GLN:CD	0.71	2.11	13	2
1:B:43:ILE:HG23	1:B:66:ILE:HG13	0.71	1.63	15	1
1:A:57:THR:HA	1:A:65:PHE:O	0.71	1.86	5	16
1:A:101:LEU:HD12	1:B:25:GLN:NE2	0.71	2.01	5	3
1:B:22:VAL:O	1:B:37:VAL:HG12	0.71	1.86	6	5
1:A:22:VAL:O	1:A:24:VAL:HG13	0.71	1.86	18	1
1:B:58:ILE:HG22	1:B:60:ILE:HG23	0.70	1.62	20	6
1:B:8:LYS:HG3	1:B:9:ASN:ND2	0.70	2.00	12	4
1:B:41:THR:HG21	1:B:68:LEU:HD13	0.70	1.60	11	7
1:A:40:LEU:HD23	1:A:66:ILE:C	0.70	2.11	14	6
1:A:54:LEU:HD12	1:A:100:PHE:CE2	0.70	2.21	15	4
1:B:37:VAL:HG11	1:B:75:VAL:HG22	0.70	1.63	4	1
1:A:28:LEU:O	1:A:32:LEU:HD12	0.70	1.86	20	2
1:B:37:VAL:HG22	1:B:73:THR:O	0.70	1.87	7	8
1:B:58:ILE:HD12	1:B:59:HIS:N	0.70	2.01	1	1
1:A:38:ILE:HD12	1:A:69:THR:CG2	0.70	2.15	18	2
1:A:24:VAL:HG22	1:A:98:ILE:HD12	0.70	1.63	10	11
1:B:97:ALA:O	1:B:101:LEU:HB3	0.70	1.87	19	19
1:A:103:THR:OG1	1:A:105:ILE:HG23	0.70	1.87	19	1
1:A:97:ALA:O	1:A:101:LEU:HB3	0.70	1.87	7	18
1:B:9:ASN:C	1:B:82:GLU:H	0.70	1.95	1	7
1:B:9:ASN:OD1	1:B:9:ASN:O	0.70	2.09	5	3
1:B:22:VAL:HG23	1:B:40:LEU:HD11	0.70	1.62	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:35:ARG:NH2	1:B:75:VAL:HG13	0.70	2.00	3	1
1:B:99:ASP:CG	1:B:105:ILE:HD12	0.70	2.12	19	1
1:A:37:VAL:HG22	1:A:73:THR:O	0.70	1.87	7	5
1:A:58:ILE:HD12	1:A:87:LEU:CD2	0.70	2.17	3	3
1:A:102:ILE:HD13	1:A:103:THR:HG23	0.70	1.63	6	1
1:A:76:PRO:O	1:A:79:ILE:HD12	0.69	1.86	16	9
1:A:6:LEU:HD12	1:A:60:ILE:HG21	0.69	1.62	18	1
1:A:72:MET:SD	1:A:101:LEU:HD21	0.69	2.26	5	4
1:A:6:LEU:CD2	1:A:60:ILE:HD13	0.69	2.17	4	2
1:A:26:SER:O	1:A:30:ASP:N	0.69	2.25	16	9
1:B:38:ILE:HG23	1:B:69:THR:HG23	0.69	1.63	7	5
1:B:31:ASN:CG	1:B:77:VAL:HG23	0.69	2.12	18	2
1:A:54:LEU:HD21	1:A:101:LEU:HD22	0.69	1.63	14	1
1:A:30:ASP:O	1:A:35:ARG:HG2	0.69	1.86	11	4
1:A:39:PRO:O	1:A:68:LEU:HB2	0.69	1.86	5	20
1:A:24:VAL:HG12	1:A:94:ILE:HG23	0.69	1.63	18	1
1:B:39:PRO:O	1:B:68:LEU:HB2	0.69	1.87	15	20
1:B:6:LEU:HD23	1:B:85:ASN:HB3	0.69	1.65	20	4
1:B:102:ILE:HG13	1:B:103:THR:HG23	0.69	1.65	2	3
1:A:4:PHE:CZ	1:A:95:ILE:HD11	0.69	2.22	14	6
1:B:6:LEU:CD1	1:B:60:ILE:HD13	0.69	2.17	14	8
1:A:19:PRO:CG	1:A:42:PRO:HD3	0.69	2.18	15	20
1:B:10:LYS:HA	1:B:82:GLU:N	0.69	2.03	2	13
1:A:8:LYS:O	1:A:81:SER:HB3	0.69	1.88	19	4
1:A:10:LYS:HA	1:A:82:GLU:N	0.69	2.03	9	6
1:A:35:ARG:CG	1:A:80:LEU:HD11	0.69	2.17	12	1
1:A:38:ILE:HD12	1:A:67:MET:HG2	0.68	1.62	1	1
1:A:58:ILE:O	1:A:64:ASP:HA	0.68	1.87	10	4
1:A:10:LYS:HD3	1:A:10:LYS:N	0.68	2.01	8	5
1:B:7:TYR:O	1:B:20:TYR:HB2	0.68	1.88	15	1
1:A:69:THR:O	1:A:101:LEU:HD13	0.68	1.88	3	3
1:A:72:MET:HE1	1:A:98:ILE:HG12	0.68	1.66	11	2
1:B:20:TYR:CG	1:B:40:LEU:HD12	0.68	2.23	15	1
1:A:24:VAL:CG2	1:A:98:ILE:HD11	0.68	2.16	18	1
1:A:67:MET:HE3	1:A:94:ILE:HD12	0.68	1.65	19	1
1:B:72:MET:CE	1:B:101:LEU:HD21	0.68	2.19	2	4
1:A:67:MET:HE1	1:A:93:GLU:HB3	0.68	1.64	20	2
1:A:10:LYS:HG2	1:A:79:ILE:CG2	0.68	2.19	13	1
1:B:102:ILE:HD13	1:B:103:THR:HG23	0.68	1.65	10	2
1:B:8:LYS:CA	1:B:20:TYR:HB3	0.68	2.19	2	4
1:A:67:MET:HE1	1:A:94:ILE:CD1	0.68	2.19	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:ILE:HD11	1:B:57:THR:HG1	0.68	1.47	18	3
1:A:58:ILE:HG22	1:A:90:PHE:CG	0.68	2.24	11	3
1:B:8:LYS:HA	1:B:20:TYR:CB	0.68	2.14	15	16
1:B:68:LEU:HD23	1:B:71:GLN:HB2	0.68	1.64	19	3
1:A:40:LEU:HD21	1:A:67:MET:SD	0.68	2.28	1	2
1:B:10:LYS:HD3	1:B:11:ASP:H	0.68	1.48	2	14
1:B:22:VAL:HG21	1:B:67:MET:HE2	0.68	1.64	14	2
1:B:98:ILE:HG13	1:B:102:ILE:HD12	0.68	1.65	4	4
1:B:69:THR:HG21	1:B:97:ALA:HB1	0.68	1.64	4	2
1:B:87:LEU:HD12	1:B:87:LEU:H	0.68	1.48	3	13
1:A:58:ILE:HD12	1:A:87:LEU:HD22	0.68	1.65	17	3
1:A:10:LYS:HD3	1:A:11:ASP:N	0.68	2.03	11	9
1:B:30:ASP:HA	1:B:35:ARG:CD	0.68	2.19	14	3
1:B:72:MET:O	1:B:73:THR:HG23	0.68	1.89	13	1
1:A:72:MET:CE	1:A:101:LEU:HD21	0.67	2.19	2	2
1:B:94:ILE:O	1:B:97:ALA:HB3	0.67	1.89	3	4
1:A:6:LEU:HD11	1:A:85:ASN:CB	0.67	2.19	20	1
1:B:26:SER:CB	1:B:29:LEU:HB2	0.67	2.19	5	20
1:B:35:ARG:HD2	1:B:37:VAL:HG13	0.67	1.64	17	1
1:A:22:VAL:O	1:A:24:VAL:HG12	0.67	1.90	3	19
1:B:6:LEU:CD2	1:B:60:ILE:HD13	0.67	2.20	18	1
1:A:102:ILE:HD12	1:A:103:THR:N	0.67	2.05	6	2
1:B:75:VAL:O	1:B:80:LEU:HD22	0.67	1.89	9	1
1:A:8:LYS:HE3	1:A:15:ALA:HB2	0.67	1.67	18	1
1:B:69:THR:CG2	1:B:101:LEU:HD22	0.67	2.20	17	11
1:A:75:VAL:HG23	1:A:79:ILE:CD1	0.67	2.18	6	3
1:A:101:LEU:HD11	1:B:25:GLN:NE2	0.67	2.04	18	3
1:A:10:LYS:HD3	1:A:11:ASP:H	0.67	1.49	20	11
1:B:36:LEU:HD11	1:B:72:MET:CG	0.67	2.20	4	2
1:B:40:LEU:HD21	1:B:58:ILE:HG13	0.67	1.64	7	3
1:A:102:ILE:HG23	1:B:25:GLN:OE1	0.67	1.90	12	1
1:B:22:VAL:O	1:B:24:VAL:HG12	0.66	1.89	14	17
1:B:10:LYS:HG3	1:B:79:ILE:O	0.66	1.90	5	4
1:B:102:ILE:HD12	1:B:103:THR:N	0.66	2.05	11	2
1:A:24:VAL:HG21	1:A:98:ILE:CD1	0.66	2.18	18	1
1:B:100:PHE:HB2	1:B:105:ILE:HG22	0.66	1.67	19	1
1:A:56:PRO:HG2	1:A:67:MET:HE2	0.66	1.66	19	3
1:B:43:ILE:HD12	1:B:57:THR:CG2	0.66	2.20	17	1
1:A:6:LEU:HD12	1:A:87:LEU:HB3	0.66	1.67	2	1
1:B:43:ILE:HD12	1:B:64:ASP:OD2	0.66	1.90	18	1
1:B:72:MET:SD	1:B:101:LEU:HD21	0.66	2.31	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:PHE:CD2	1:B:94:ILE:HD12	0.66	2.26	4	1
1:A:9:ASN:N	1:A:81:SER:OG	0.66	2.28	6	5
1:B:40:LEU:HD23	1:B:66:ILE:C	0.66	2.14	7	7
1:A:10:LYS:HG2	1:A:79:ILE:CG1	0.66	2.21	18	1
1:A:25:GLN:OE1	1:A:36:LEU:HD22	0.66	1.90	20	1
1:B:24:VAL:HB	1:B:94:ILE:HG23	0.66	1.68	7	4
1:B:37:VAL:CG1	1:B:75:VAL:HG22	0.66	2.21	4	1
1:B:103:THR:HG22	1:B:105:ILE:HG23	0.66	1.67	13	3
1:A:102:ILE:HG13	1:A:103:THR:HG23	0.66	1.66	3	3
1:B:72:MET:HE3	1:B:102:ILE:HD11	0.66	1.67	5	1
1:B:19:PRO:CG	1:B:42:PRO:HD3	0.66	2.21	15	19
1:A:98:ILE:HG13	1:A:102:ILE:HD12	0.66	1.66	18	3
1:A:103:THR:HG22	1:A:105:ILE:HG23	0.65	1.68	12	1
1:B:35:ARG:NH2	1:B:80:LEU:HD22	0.65	2.06	13	2
1:B:20:TYR:N	1:B:20:TYR:CD1	0.65	2.64	12	20
1:A:10:LYS:CG	1:A:79:ILE:HB	0.65	2.21	2	10
1:A:36:LEU:HD22	1:A:74:SER:HB3	0.65	1.67	18	1
1:B:69:THR:O	1:B:101:LEU:HD13	0.65	1.91	8	4
1:B:41:THR:O	1:B:66:ILE:HD12	0.65	1.91	7	19
1:B:92:ASN:HA	1:B:95:ILE:HD12	0.65	1.68	2	11
1:B:22:VAL:CG2	1:B:67:MET:HE3	0.65	2.20	13	6
1:B:98:ILE:HA	1:B:101:LEU:HD23	0.65	1.68	8	9
1:A:54:LEU:CD2	1:A:69:THR:HG23	0.65	2.21	3	1
1:B:76:PRO:HD2	1:B:79:ILE:HD11	0.65	1.67	20	6
1:B:58:ILE:HD11	1:B:67:MET:SD	0.65	2.32	18	2
1:A:7:TYR:CD2	1:A:80:LEU:HD12	0.65	2.27	7	5
1:A:73:THR:HG22	1:B:73:THR:OG1	0.65	1.91	5	1
1:A:103:THR:HG1	1:A:105:ILE:HG23	0.65	1.51	19	1
1:A:79:ILE:O	1:A:81:SER:N	0.65	2.30	2	11
1:B:79:ILE:O	1:B:81:SER:N	0.65	2.29	10	12
1:A:25:GLN:OE1	1:B:102:ILE:HG23	0.65	1.92	18	1
1:B:10:LYS:N	1:B:82:GLU:H	0.65	1.90	5	8
1:A:6:LEU:HD23	1:A:87:LEU:N	0.65	2.07	20	1
1:A:20:TYR:CD1	1:A:20:TYR:N	0.65	2.65	4	20
1:A:92:ASN:O	1:A:96:ALA:N	0.64	2.29	20	20
1:B:23:ASP:OD1	1:B:80:LEU:HD21	0.64	1.93	1	1
1:B:33:ASN:O	1:B:34:THR:HG22	0.64	1.92	9	9
1:A:92:ASN:HA	1:A:95:ILE:HD12	0.64	1.69	7	9
1:A:22:VAL:HG21	1:A:67:MET:HE3	0.64	1.68	7	2
1:B:6:LEU:HD13	1:B:60:ILE:HD13	0.64	1.68	16	5
1:A:98:ILE:HA	1:A:101:LEU:HD23	0.64	1.68	3	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:HD21	1:B:67:MET:CE	0.64	2.13	8	1
1:B:8:LYS:O	1:B:81:SER:HB3	0.64	1.93	13	2
1:B:10:LYS:HD3	1:B:11:ASP:N	0.64	2.06	2	12
1:B:92:ASN:O	1:B:96:ALA:N	0.64	2.30	13	20
1:A:8:LYS:O	1:A:10:LYS:N	0.64	2.31	5	1
1:B:58:ILE:HD13	1:B:90:PHE:CD1	0.64	2.27	18	3
1:B:10:LYS:H	1:B:81:SER:HA	0.64	1.52	7	5
1:B:2:SER:O	1:B:3:GLN:CB	0.64	2.46	8	7
1:B:40:LEU:HD23	1:B:67:MET:CG	0.64	2.22	15	4
1:A:5:THR:HB	1:A:7:TYR:CZ	0.64	2.26	13	20
1:A:9:ASN:O	1:A:10:LYS:C	0.64	2.39	7	18
1:A:9:ASN:O	1:A:11:ASP:N	0.64	2.31	7	19
1:B:9:ASN:ND2	1:B:15:ALA:HB2	0.64	2.07	7	1
1:B:10:LYS:N	1:B:10:LYS:HD3	0.64	2.07	12	9
1:B:75:VAL:HG23	1:B:79:ILE:CD1	0.64	2.21	3	2
1:B:101:LEU:HD13	1:B:102:ILE:CG1	0.64	2.23	14	3
1:A:20:TYR:OH	1:A:65:PHE:CE2	0.64	2.51	6	5
1:B:24:VAL:CG2	1:B:98:ILE:HD12	0.64	2.23	5	3
1:A:10:LYS:N	1:A:10:LYS:HD3	0.64	2.08	9	5
1:A:9:ASN:OD1	1:A:12:LYS:HA	0.64	1.92	3	1
1:B:58:ILE:HG21	1:B:87:LEU:CD2	0.64	2.23	18	5
1:A:72:MET:HE1	1:A:102:ILE:CD1	0.64	2.23	18	2
1:A:94:ILE:O	1:A:97:ALA:HB3	0.64	1.94	3	4
1:A:10:LYS:CG	1:A:79:ILE:CG1	0.64	2.76	18	7
1:B:60:ILE:HD12	1:B:62:GLU:HB2	0.64	1.69	12	2
1:A:75:VAL:HG13	1:A:80:LEU:HD22	0.64	1.69	9	1
1:B:9:ASN:O	1:B:10:LYS:C	0.63	2.40	13	20
1:B:41:THR:OG1	1:B:42:PRO:HD2	0.63	1.92	20	20
1:B:20:TYR:OH	1:B:65:PHE:CG	0.63	2.47	6	3
1:A:54:LEU:HD13	1:A:54:LEU:O	0.63	1.92	4	1
1:A:102:ILE:HD12	1:A:103:THR:HG23	0.63	1.69	4	2
1:A:38:ILE:HG13	1:A:72:MET:HE2	0.63	1.71	6	2
1:A:23:ASP:OD2	1:A:80:LEU:HD21	0.63	1.93	11	3
1:B:40:LEU:CG	1:B:67:MET:HE3	0.63	2.23	14	1
1:B:9:ASN:O	1:B:11:ASP:N	0.63	2.31	13	20
1:B:10:LYS:CG	1:B:79:ILE:HB	0.63	2.24	18	8
1:B:58:ILE:HG23	1:B:60:ILE:HG23	0.63	1.71	4	3
1:A:9:ASN:N	1:A:19:PRO:O	0.63	2.32	1	14
1:A:26:SER:CB	1:A:29:LEU:HB2	0.63	2.23	13	19
1:A:41:THR:OG1	1:A:42:PRO:HD2	0.63	1.94	2	20
1:B:43:ILE:CD1	1:B:57:THR:HG22	0.63	2.23	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD11	1:A:72:MET:HE3	0.63	1.69	5	2
1:A:102:ILE:HD12	1:B:102:ILE:HD13	0.63	1.70	10	1
1:A:40:LEU:HD22	1:A:58:ILE:HD12	0.63	1.71	13	3
1:B:30:ASP:O	1:B:35:ARG:HD3	0.63	1.93	19	1
1:A:69:THR:CG2	1:A:101:LEU:HD22	0.63	2.23	1	12
1:A:4:PHE:HD1	1:A:94:ILE:HD12	0.63	1.54	3	1
1:A:87:LEU:H	1:A:87:LEU:HD12	0.63	1.53	9	11
1:B:8:LYS:O	1:B:9:ASN:O	0.63	2.17	3	9
1:B:56:PRO:HG2	1:B:67:MET:HE3	0.63	1.70	11	2
1:B:10:LYS:HD2	1:B:11:ASP:N	0.63	2.08	5	1
1:B:19:PRO:HB2	1:B:20:TYR:CE1	0.63	2.29	1	17
1:B:20:TYR:OH	1:B:65:PHE:CD1	0.63	2.52	17	11
1:B:58:ILE:N	1:B:58:ILE:HD12	0.63	2.08	12	2
1:A:25:GLN:CD	1:B:101:LEU:HD12	0.63	2.19	9	2
1:A:9:ASN:C	1:A:82:GLU:H	0.63	2.02	8	7
1:B:9:ASN:O	1:B:9:ASN:OD1	0.63	2.17	3	2
1:B:10:LYS:HG2	1:B:79:ILE:CB	0.63	2.24	6	3
1:B:6:LEU:HG	1:B:87:LEU:HD13	0.63	1.70	7	2
1:B:58:ILE:HG23	1:B:67:MET:HE1	0.63	1.71	9	1
1:B:4:PHE:HD1	1:B:94:ILE:HD12	0.62	1.54	10	2
1:A:40:LEU:HD21	1:A:58:ILE:HG13	0.62	1.70	14	3
1:A:6:LEU:HG	1:A:60:ILE:HD13	0.62	1.68	15	1
1:B:7:TYR:O	1:B:20:TYR:HB3	0.62	1.94	5	17
1:A:57:THR:HG1	1:A:66:ILE:HG23	0.62	1.53	20	4
1:A:35:ARG:NH2	1:A:80:LEU:HD22	0.62	2.09	14	2
1:A:31:ASN:OD1	1:A:77:VAL:HG23	0.62	1.94	8	2
1:B:3:GLN:HA	1:B:35:ARG:NH1	0.62	2.09	10	1
1:B:35:ARG:HA	1:B:35:ARG:CZ	0.62	2.23	18	3
1:B:6:LEU:HD11	1:B:60:ILE:HG21	0.62	1.71	9	2
1:B:35:ARG:O	1:B:74:SER:HA	0.62	1.94	11	3
1:A:101:LEU:HD13	1:A:102:ILE:CG1	0.62	2.24	15	1
1:A:7:TYR:HB3	1:A:81:SER:HB2	0.62	1.71	12	5
1:B:80:LEU:O	1:B:81:SER:O	0.62	2.16	18	10
1:B:98:ILE:HG23	1:B:102:ILE:CG1	0.62	2.24	10	2
1:B:10:LYS:CG	1:B:79:ILE:HA	0.62	2.24	2	6
1:B:42:PRO:HG3	1:B:45:LEU:HD23	0.62	1.71	2	2
1:B:35:ARG:HD2	1:B:80:LEU:HD21	0.62	1.72	9	1
1:A:40:LEU:HG	1:A:67:MET:HG2	0.62	1.72	3	1
1:A:29:LEU:CD2	1:A:32:LEU:HD22	0.62	2.24	12	2
1:A:36:LEU:HD21	1:B:72:MET:HE1	0.62	1.69	6	1
1:B:43:ILE:HD11	1:B:57:THR:CG2	0.62	2.25	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HD12	1:A:58:ILE:N	0.62	2.10	2	2
1:B:6:LEU:HD13	1:B:87:LEU:HD13	0.62	1.72	19	2
1:A:7:TYR:CD2	1:A:80:LEU:HD11	0.62	2.29	19	2
1:A:58:ILE:CD1	1:A:60:ILE:N	0.62	2.63	10	2
1:A:41:THR:HG21	1:A:68:LEU:HD13	0.61	1.71	13	8
1:B:54:LEU:HD12	1:B:100:PHE:CE2	0.61	2.30	13	3
1:A:34:THR:HG22	1:A:76:PRO:HA	0.61	1.71	9	3
1:B:31:ASN:OD1	1:B:77:VAL:HG23	0.61	1.95	14	4
1:A:80:LEU:O	1:A:81:SER:O	0.61	2.18	13	9
1:B:38:ILE:O	1:B:38:ILE:HG23	0.61	1.95	2	2
1:A:102:ILE:HG21	1:B:102:ILE:CD1	0.61	2.24	9	1
1:A:75:VAL:HG12	1:A:79:ILE:CD1	0.61	2.26	20	4
1:A:79:ILE:O	1:A:80:LEU:C	0.61	2.43	16	4
1:A:30:ASP:O	1:A:35:ARG:CB	0.61	2.47	14	6
1:B:10:LYS:CG	1:B:79:ILE:HG12	0.61	2.26	1	6
1:B:7:TYR:O	1:B:20:TYR:CB	0.61	2.48	2	12
1:B:9:ASN:N	1:B:19:PRO:O	0.61	2.34	16	18
1:A:10:LYS:CB	1:A:79:ILE:HG12	0.61	2.26	18	2
1:A:99:ASP:O	1:A:105:ILE:HD13	0.61	1.94	14	1
1:B:30:ASP:O	1:B:34:THR:O	0.61	2.18	8	4
1:B:53:HIS:C	1:B:54:LEU:HD12	0.61	2.20	1	1
1:A:98:ILE:HA	1:A:102:ILE:HG23	0.61	1.70	17	4
1:B:72:MET:HE1	1:B:101:LEU:CD2	0.61	2.15	19	2
1:B:41:THR:HG21	1:B:68:LEU:HD23	0.61	1.72	17	2
1:A:38:ILE:CD1	1:A:69:THR:HG23	0.61	2.23	18	1
1:A:19:PRO:HB2	1:A:20:TYR:CE1	0.61	2.31	14	20
1:A:21:PHE:CD2	1:A:75:VAL:HG21	0.61	2.30	15	2
1:A:41:THR:O	1:A:66:ILE:HD12	0.61	1.94	13	20
1:A:67:MET:HE1	1:A:93:GLU:C	0.61	2.21	14	3
1:A:38:ILE:CG1	1:A:72:MET:HE2	0.61	2.26	14	1
1:A:54:LEU:HD11	1:A:101:LEU:HD13	0.61	1.71	18	1
1:A:42:PRO:CG	1:A:45:LEU:HD12	0.61	2.25	8	9
1:B:45:LEU:HD12	1:B:45:LEU:C	0.61	2.21	2	2
1:A:43:ILE:HD12	1:A:64:ASP:HB3	0.61	1.72	3	2
1:A:10:LYS:HA	1:A:81:SER:HA	0.61	1.73	1	2
1:A:99:ASP:HA	1:A:103:THR:HG23	0.61	1.71	1	6
1:A:58:ILE:HD12	1:A:59:HIS:CA	0.61	2.25	19	2
1:A:10:LYS:CA	1:A:81:SER:HA	0.60	2.26	1	2
1:B:8:LYS:CE	1:B:15:ALA:HB2	0.60	2.26	2	1
1:B:79:ILE:O	1:B:80:LEU:C	0.60	2.44	3	7
1:A:5:THR:CB	1:A:7:TYR:CE1	0.60	2.84	12	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:TYR:O	1:A:20:TYR:HB3	0.60	1.96	17	15
1:A:69:THR:OG1	1:A:72:MET:HE2	0.60	1.95	2	1
1:A:97:ALA:O	1:A:101:LEU:CB	0.60	2.48	10	1
1:B:29:LEU:HD23	1:B:32:LEU:HG	0.60	1.72	5	2
1:B:8:LYS:O	1:B:9:ASN:C	0.60	2.43	17	18
1:A:8:LYS:HE2	1:A:84:VAL:HG13	0.60	1.70	5	1
1:B:28:LEU:O	1:B:32:LEU:HD13	0.60	1.97	6	3
1:B:6:LEU:CD1	1:B:87:LEU:HD13	0.60	2.26	13	2
1:B:98:ILE:HA	1:B:102:ILE:HG23	0.60	1.72	2	4
1:A:58:ILE:CD1	1:A:58:ILE:C	0.60	2.69	19	1
1:B:25:GLN:NE2	1:B:36:LEU:HD23	0.60	2.11	20	1
1:A:33:ASN:O	1:A:34:THR:HG22	0.60	1.97	13	10
1:B:58:ILE:CD1	1:B:60:ILE:HG23	0.60	2.05	1	1
1:A:67:MET:HE1	1:A:94:ILE:CG1	0.60	2.25	2	2
1:A:76:PRO:HD2	1:A:79:ILE:HD11	0.60	1.72	15	6
1:A:10:LYS:HG2	1:A:79:ILE:HA	0.60	1.73	12	6
1:B:10:LYS:HG2	1:B:79:ILE:CG2	0.60	2.25	20	3
1:B:43:ILE:HG23	1:B:66:ILE:CG1	0.60	2.26	15	1
1:A:20:TYR:CD1	1:A:40:LEU:HD13	0.60	2.31	16	1
1:B:10:LYS:HG2	1:B:79:ILE:HA	0.60	1.72	5	7
1:B:58:ILE:C	1:B:58:ILE:CD1	0.60	2.71	1	1
1:B:58:ILE:O	1:B:64:ASP:HA	0.60	1.96	1	6
1:A:24:VAL:O	1:A:25:GLN:CB	0.60	2.48	2	6
1:B:58:ILE:HG22	1:B:90:PHE:CD1	0.60	2.31	6	2
1:B:9:ASN:OD1	1:B:15:ALA:N	0.60	2.35	12	5
1:A:9:ASN:C	1:A:10:LYS:HD2	0.60	2.21	18	2
1:A:2:SER:O	1:A:3:GLN:CB	0.60	2.50	20	10
1:B:30:ASP:O	1:B:35:ARG:CB	0.60	2.49	17	2
1:A:22:VAL:HG23	1:A:40:LEU:HD11	0.60	1.73	4	1
1:B:99:ASP:HA	1:B:103:THR:OG1	0.60	1.95	11	2
1:B:28:LEU:HD12	1:B:28:LEU:N	0.59	2.12	19	6
1:B:6:LEU:HD13	1:B:87:LEU:HD21	0.59	1.72	18	3
1:A:23:ASP:OD1	1:A:80:LEU:HD21	0.59	1.96	15	3
1:A:10:LYS:HG2	1:A:79:ILE:CB	0.59	2.27	13	1
1:B:58:ILE:HG12	1:B:90:PHE:CD2	0.59	2.32	16	3
1:A:38:ILE:HG23	1:A:69:THR:HG23	0.59	1.74	15	7
1:B:5:THR:HB	1:B:7:TYR:CZ	0.59	2.32	1	20
1:B:33:ASN:O	1:B:34:THR:CG2	0.59	2.51	6	12
1:B:19:PRO:HG3	1:B:42:PRO:HD3	0.59	1.74	6	13
1:B:9:ASN:ND2	1:B:19:PRO:HA	0.59	2.12	10	5
1:A:10:LYS:H	1:A:81:SER:HA	0.59	1.56	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:ILE:HG23	1:B:48:LYS:CG	0.59	2.27	17	1
1:A:20:TYR:O	1:A:40:LEU:N	0.59	2.36	14	15
1:A:80:LEU:O	1:A:81:SER:C	0.59	2.45	16	10
1:B:7:TYR:CD2	1:B:80:LEU:HD22	0.59	2.32	14	1
1:B:57:THR:CG2	1:B:58:ILE:N	0.59	2.66	5	15
1:B:9:ASN:N	1:B:81:SER:OG	0.59	2.35	16	4
1:A:79:ILE:O	1:A:79:ILE:CG1	0.59	2.47	18	5
1:A:58:ILE:HG13	1:A:90:PHE:CE1	0.59	2.33	18	3
1:B:77:VAL:HA	1:B:80:LEU:HD23	0.59	1.75	18	1
1:A:5:THR:HG23	1:A:86:GLU:HG2	0.59	1.74	8	1
1:A:75:VAL:CG1	1:A:79:ILE:HD13	0.59	2.28	11	1
1:A:8:LYS:O	1:A:9:ASN:C	0.59	2.45	4	13
1:A:57:THR:CG2	1:A:58:ILE:N	0.59	2.65	19	14
1:A:58:ILE:HD13	1:A:58:ILE:H	0.59	1.58	13	6
1:B:24:VAL:HG21	1:B:98:ILE:HD13	0.59	1.75	3	9
1:A:30:ASP:O	1:A:34:THR:O	0.59	2.21	20	6
1:B:75:VAL:HG12	1:B:79:ILE:CD1	0.59	2.27	18	3
1:B:38:ILE:CD1	1:B:67:MET:HB3	0.59	2.28	2	3
1:B:38:ILE:HD13	1:B:67:MET:HB3	0.59	1.75	2	1
1:A:54:LEU:HD21	1:A:100:PHE:CD2	0.59	2.31	6	1
1:A:99:ASP:HA	1:A:103:THR:OG1	0.59	1.97	6	1
1:A:25:GLN:HE22	1:B:101:LEU:HD11	0.59	1.58	12	1
1:B:36:LEU:HD21	1:B:72:MET:SD	0.59	2.38	4	2
1:A:35:ARG:NE	1:A:80:LEU:HD22	0.59	2.13	17	1
1:B:28:LEU:O	1:B:32:LEU:HD23	0.59	1.98	5	1
1:B:67:MET:HE1	1:B:94:ILE:HG23	0.59	1.74	10	1
1:A:6:LEU:HD23	1:A:85:ASN:HB3	0.58	1.74	1	3
1:B:10:LYS:HD2	1:B:11:ASP:H	0.58	1.56	5	1
1:A:69:THR:HB	1:A:101:LEU:HD13	0.58	1.74	1	2
1:B:58:ILE:HG23	1:B:90:PHE:CD1	0.58	2.33	15	1
1:A:38:ILE:HD13	1:A:97:ALA:CB	0.58	2.27	3	2
1:B:38:ILE:HD13	1:B:97:ALA:CB	0.58	2.27	16	3
1:A:2:SER:O	1:A:30:ASP:HB2	0.58	1.98	11	4
1:A:6:LEU:HD13	1:A:6:LEU:O	0.58	1.99	15	2
1:B:22:VAL:CG2	1:B:40:LEU:HD11	0.58	2.28	12	2
1:B:24:VAL:CG2	1:B:98:ILE:HD13	0.58	2.27	7	10
1:A:31:ASN:HD21	1:A:77:VAL:HG23	0.58	1.59	13	1
1:B:24:VAL:HG23	1:B:24:VAL:O	0.58	1.98	15	1
1:A:6:LEU:HD11	1:A:85:ASN:HB3	0.58	1.75	20	1
1:A:20:TYR:C	1:A:40:LEU:HD12	0.58	2.24	16	2
1:A:29:LEU:HD13	1:B:54:LEU:HD12	0.58	1.75	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:9:ASN:HD21	1:B:15:ALA:HB2	0.58	1.58	7	1
1:B:40:LEU:HA	1:B:66:ILE:O	0.58	1.98	15	1
1:B:75:VAL:CG2	1:B:79:ILE:HG23	0.58	2.28	17	1
1:A:46:LEU:HD21	1:A:68:LEU:CD1	0.58	2.29	18	1
1:A:72:MET:HE2	1:B:36:LEU:HD21	0.58	1.76	1	1
1:B:5:THR:CB	1:B:7:TYR:CE1	0.58	2.86	17	17
1:A:24:VAL:HG11	1:A:38:ILE:CD1	0.58	2.29	17	9
1:B:40:LEU:CD2	1:B:58:ILE:HD11	0.58	2.29	3	1
1:A:67:MET:HE1	1:A:94:ILE:HG23	0.58	1.74	4	1
1:A:55:CYS:SG	1:A:68:LEU:HD23	0.58	2.38	5	1
1:A:24:VAL:HG11	1:A:94:ILE:HG22	0.58	1.75	2	6
1:A:99:ASP:O	1:A:103:THR:OG1	0.58	2.21	11	5
1:A:87:LEU:N	1:A:87:LEU:CD2	0.58	2.66	4	3
1:A:29:LEU:HD13	1:B:70:GLN:CG	0.58	2.28	10	1
1:A:28:LEU:N	1:A:28:LEU:HD12	0.58	2.13	7	7
1:A:29:LEU:HA	1:A:32:LEU:HD23	0.58	1.76	6	1
1:A:72:MET:HE1	1:A:98:ILE:CG1	0.58	2.27	11	1
1:A:20:TYR:OH	1:A:60:ILE:HD11	0.58	1.99	16	1
1:A:33:ASN:O	1:A:34:THR:CG2	0.58	2.52	17	10
1:B:6:LEU:HD13	1:B:87:LEU:HG	0.58	1.76	6	1
1:A:72:MET:SD	1:A:102:ILE:HD11	0.58	2.39	18	2
1:A:6:LEU:HG	1:A:87:LEU:HD13	0.58	1.74	18	1
1:A:105:ILE:HD12	1:A:105:ILE:OXT	0.58	1.99	1	2
1:A:25:GLN:OE1	1:B:101:LEU:HD11	0.58	1.99	15	2
1:A:10:LYS:CG	1:A:79:ILE:HG12	0.58	2.29	11	7
1:A:58:ILE:N	1:A:58:ILE:HD13	0.58	2.13	12	5
1:A:98:ILE:CG2	1:A:102:ILE:HD11	0.58	2.28	16	2
1:B:10:LYS:HB3	1:B:79:ILE:O	0.58	1.98	7	2
1:B:80:LEU:O	1:B:81:SER:C	0.57	2.46	16	8
1:B:30:ASP:O	1:B:35:ARG:HD2	0.57	1.99	8	1
1:A:58:ILE:HD13	1:A:58:ILE:N	0.57	2.13	13	2
1:B:64:ASP:O	1:B:65:PHE:CD1	0.57	2.58	3	14
1:A:45:LEU:HD12	1:A:45:LEU:C	0.57	2.23	4	1
1:B:2:SER:CB	1:B:30:ASP:HB2	0.57	2.29	19	1
1:B:20:TYR:CG	1:B:40:LEU:HD13	0.57	2.34	6	2
1:A:25:GLN:HB2	1:A:36:LEU:CB	0.57	2.29	17	7
1:A:75:VAL:HG23	1:A:75:VAL:O	0.57	1.99	1	5
1:B:20:TYR:O	1:B:40:LEU:N	0.57	2.38	4	15
1:A:24:VAL:HG21	1:A:98:ILE:HD13	0.57	1.75	12	4
1:A:97:ALA:O	1:A:101:LEU:N	0.57	2.32	10	5
1:A:10:LYS:HD2	1:A:79:ILE:CG1	0.57	2.29	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ILE:O	1:A:102:ILE:HB	0.57	2.00	20	10
1:A:67:MET:HE2	1:A:94:ILE:CG1	0.57	2.30	10	1
1:A:40:LEU:HD22	1:A:58:ILE:CD1	0.57	2.30	1	3
1:B:36:LEU:HD13	1:B:36:LEU:C	0.57	2.24	7	2
1:B:42:PRO:CG	1:B:45:LEU:HD12	0.57	2.29	8	4
1:A:21:PHE:CD2	1:A:75:VAL:HG11	0.57	2.35	1	6
1:A:35:ARG:HA	1:A:35:ARG:CZ	0.57	2.29	3	2
1:B:58:ILE:N	1:B:58:ILE:HD13	0.57	2.15	9	7
1:A:7:TYR:CD2	1:A:80:LEU:CD1	0.57	2.87	20	5
1:A:67:MET:HE1	1:A:93:GLU:O	0.57	2.00	14	1
1:A:25:GLN:NE2	1:B:101:LEU:HD12	0.57	2.14	1	1
1:A:58:ILE:HA	1:A:90:PHE:CE2	0.57	2.34	2	2
1:B:10:LYS:CD	1:B:79:ILE:HG13	0.57	2.30	17	6
1:B:67:MET:HE1	1:B:93:GLU:HB3	0.57	1.77	18	2
1:B:6:LEU:HD12	1:B:85:ASN:HB2	0.57	1.76	4	1
1:B:23:ASP:N	1:B:37:VAL:HG12	0.57	2.15	19	2
1:B:67:MET:HE1	1:B:93:GLU:CG	0.57	2.29	3	1
1:A:87:LEU:N	1:A:87:LEU:HD22	0.57	2.14	4	1
1:B:30:ASP:O	1:B:35:ARG:HG2	0.57	2.00	12	1
1:A:24:VAL:CG2	1:A:98:ILE:HD12	0.56	2.31	1	6
1:A:58:ILE:HG21	1:A:87:LEU:CD2	0.56	2.27	17	3
1:B:36:LEU:CD2	1:B:72:MET:HE2	0.56	2.29	10	1
1:A:7:TYR:O	1:A:20:TYR:CB	0.56	2.53	16	10
1:A:19:PRO:HG3	1:A:42:PRO:HD3	0.56	1.76	5	11
1:B:79:ILE:O	1:B:79:ILE:CG1	0.56	2.52	1	7
1:B:99:ASP:HA	1:B:103:THR:HG23	0.56	1.77	1	4
1:A:102:ILE:CG2	1:B:102:ILE:HD13	0.56	2.30	8	1
1:B:62:GLU:OE1	1:B:84:VAL:HG21	0.56	2.00	10	1
1:A:43:ILE:HD11	1:A:57:THR:HG21	0.56	1.76	19	1
1:A:20:TYR:OH	1:A:65:PHE:CZ	0.56	2.59	10	12
1:A:80:LEU:HD12	1:A:80:LEU:O	0.56	2.00	10	2
1:A:19:PRO:HG2	1:A:42:PRO:HD3	0.56	1.76	2	5
1:A:69:THR:OG1	1:A:101:LEU:CD2	0.56	2.53	16	3
1:B:69:THR:HG1	1:B:101:LEU:HD22	0.56	1.58	2	2
1:A:7:TYR:C	1:A:81:SER:CB	0.56	2.78	4	6
1:A:58:ILE:HD13	1:A:90:PHE:CG	0.56	2.35	4	1
1:B:54:LEU:HD21	1:B:69:THR:CG2	0.56	2.28	12	1
1:B:40:LEU:HD11	1:B:67:MET:CE	0.56	2.31	14	1
1:B:43:ILE:HG23	1:B:64:ASP:OD1	0.56	2.00	16	1
1:A:35:ARG:NH1	1:A:75:VAL:O	0.56	2.39	19	3
1:B:72:MET:CE	1:B:102:ILE:HD11	0.56	2.31	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:N	1:A:28:LEU:HD22	0.56	2.16	4	10
1:A:10:LYS:CG	1:A:79:ILE:HA	0.56	2.30	10	5
1:B:75:VAL:HG13	1:B:79:ILE:CD1	0.56	2.31	8	1
1:B:67:MET:HE2	1:B:93:GLU:OE1	0.56	2.00	20	1
1:B:10:LYS:HB3	1:B:79:ILE:CB	0.56	2.31	15	7
1:B:38:ILE:HG12	1:B:72:MET:HE1	0.56	1.78	8	1
1:B:54:LEU:HD23	1:B:69:THR:CG2	0.56	2.18	8	1
1:B:9:ASN:CG	1:B:19:PRO:O	0.56	2.49	15	1
1:A:8:LYS:HG3	1:A:19:PRO:O	0.56	1.99	19	13
1:B:30:ASP:O	1:B:35:ARG:HG3	0.56	2.00	9	2
1:A:98:ILE:O	1:A:102:ILE:CG1	0.56	2.54	17	5
1:B:8:LYS:HB3	1:B:84:VAL:HG13	0.56	1.78	6	4
1:B:10:LYS:CB	1:B:79:ILE:HG12	0.56	2.31	7	1
1:A:36:LEU:HD22	1:A:74:SER:CB	0.56	2.30	18	1
1:B:28:LEU:N	1:B:28:LEU:HD22	0.56	2.16	20	8
1:A:72:MET:HE1	1:A:102:ILE:HD11	0.56	1.75	2	2
1:B:22:VAL:HG21	1:B:67:MET:SD	0.56	2.40	4	1
1:A:23:ASP:OD1	1:A:80:LEU:HD11	0.56	2.00	11	3
1:A:67:MET:HE1	1:A:94:ILE:HD11	0.56	1.77	17	2
1:A:25:GLN:CD	1:A:36:LEU:HB2	0.56	2.25	17	1
1:A:38:ILE:HD13	1:A:72:MET:HG3	0.56	1.76	20	1
1:B:40:LEU:HD22	1:B:65:PHE:HB2	0.56	1.78	1	1
1:A:96:ALA:O	1:A:100:PHE:N	0.56	2.38	20	10
1:B:40:LEU:HD21	1:B:58:ILE:HD11	0.56	1.77	3	1
1:B:38:ILE:HG23	1:B:69:THR:CG2	0.56	2.31	7	1
1:A:58:ILE:HG12	1:A:87:LEU:HD12	0.56	1.77	20	1
1:A:67:MET:HE1	1:A:93:GLU:CB	0.56	2.31	20	1
1:A:8:LYS:HA	1:A:20:TYR:CB	0.56	2.27	16	18
1:A:21:PHE:HA	1:A:39:PRO:HA	0.56	1.78	18	20
1:B:9:ASN:ND2	1:B:15:ALA:N	0.56	2.54	10	4
1:A:26:SER:O	1:A:30:ASP:CB	0.56	2.54	20	7
1:B:27:ASP:OD1	1:B:28:LEU:HD22	0.56	2.01	6	1
1:A:101:LEU:HD23	1:A:102:ILE:HG13	0.56	1.77	20	1
1:A:5:THR:CB	1:A:7:TYR:CZ	0.55	2.89	13	19
1:A:8:LYS:O	1:A:81:SER:CB	0.55	2.54	3	6
1:B:21:PHE:HA	1:B:39:PRO:HA	0.55	1.78	7	18
1:B:6:LEU:HB2	1:B:87:LEU:HD22	0.55	1.76	2	4
1:B:36:LEU:HD21	1:B:72:MET:HE2	0.55	1.78	10	1
1:A:75:VAL:HG13	1:A:79:ILE:CD1	0.55	2.32	13	1
1:A:3:GLN:O	1:A:4:PHE:HB2	0.55	2.00	12	5
1:A:20:TYR:HB2	1:A:40:LEU:CD1	0.55	2.31	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:30:ASP:HA	1:B:35:ARG:NH1	0.55	2.16	8	1
1:A:58:ILE:C	1:A:58:ILE:CD1	0.55	2.74	10	1
1:B:40:LEU:HD21	1:B:67:MET:HE3	0.55	1.77	14	1
1:A:88:SER:O	1:A:91:ARG:CG	0.55	2.54	10	20
1:A:58:ILE:CG2	1:A:59:HIS:N	0.55	2.69	5	3
1:A:54:LEU:HD11	1:A:101:LEU:HB2	0.55	1.78	8	4
1:A:10:LYS:HG3	1:A:79:ILE:HG12	0.55	1.77	11	3
1:A:2:SER:OG	1:A:80:LEU:HD21	0.55	2.01	11	1
1:A:92:ASN:O	1:A:95:ILE:N	0.55	2.40	20	18
1:A:9:ASN:ND2	1:A:21:PHE:CE1	0.55	2.75	18	3
1:B:35:ARG:HG3	1:B:80:LEU:HD23	0.55	1.79	4	1
1:A:21:PHE:CD2	1:A:81:SER:OG	0.55	2.59	14	2
1:A:10:LYS:CB	1:A:79:ILE:HG22	0.55	2.31	17	4
1:B:38:ILE:HD11	1:B:67:MET:HB3	0.55	1.78	18	1
1:B:98:ILE:O	1:B:102:ILE:CG1	0.55	2.54	17	4
1:B:76:PRO:CD	1:B:79:ILE:HD11	0.55	2.31	20	5
1:B:60:ILE:HD11	1:B:65:PHE:CD2	0.55	2.36	20	2
1:B:69:THR:OG1	1:B:101:LEU:CD2	0.55	2.55	12	1
1:A:98:ILE:HG23	1:A:102:ILE:HD12	0.55	1.79	7	4
1:B:3:GLN:O	1:B:4:PHE:HB2	0.55	2.01	13	7
1:A:58:ILE:HG12	1:A:90:PHE:CD2	0.55	2.37	20	3
1:B:10:LYS:CG	1:B:79:ILE:CG1	0.55	2.84	12	7
1:B:88:SER:O	1:B:91:ARG:CG	0.55	2.55	19	20
1:A:7:TYR:CZ	1:A:23:ASP:CG	0.55	2.85	8	7
1:B:67:MET:HE1	1:B:94:ILE:CG1	0.55	2.31	7	3
1:A:25:GLN:CG	1:A:36:LEU:HB2	0.55	2.32	17	6
1:A:36:LEU:HD13	1:B:72:MET:HE2	0.55	1.77	3	1
1:A:102:ILE:CG1	1:A:103:THR:HG23	0.55	2.31	11	2
1:A:29:LEU:CD1	1:B:54:LEU:HD22	0.55	2.31	5	1
1:A:38:ILE:CD1	1:A:94:ILE:HG23	0.55	2.32	14	4
1:A:26:SER:HB3	1:A:29:LEU:HB2	0.55	1.79	14	13
1:A:17:THR:HG22	1:A:18:TYR:CE1	0.55	2.37	4	8
1:A:8:LYS:HD2	1:A:8:LYS:C	0.55	2.27	5	1
1:A:5:THR:HG23	1:A:86:GLU:HA	0.55	1.77	20	1
1:B:9:ASN:H	1:B:20:TYR:HA	0.54	1.62	7	4
1:A:41:THR:OG1	1:A:46:LEU:HD12	0.54	2.02	4	1
1:B:37:VAL:HG11	1:B:75:VAL:CG2	0.54	2.32	4	1
1:A:6:LEU:HD23	1:A:84:VAL:HG23	0.54	1.78	5	1
1:B:22:VAL:CG2	1:B:40:LEU:HD21	0.54	2.32	6	1
1:B:103:THR:HG22	1:B:105:ILE:H	0.54	1.61	7	1
1:A:10:LYS:CD	1:A:11:ASP:H	0.54	2.15	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:ALA:HA	1:B:18:TYR:C	0.54	2.27	9	20
1:B:25:GLN:HB2	1:B:36:LEU:HB3	0.54	1.79	1	6
1:B:38:ILE:HG21	1:B:67:MET:HE2	0.54	1.79	2	1
1:A:64:ASP:O	1:A:65:PHE:CD1	0.54	2.60	9	10
1:B:22:VAL:O	1:B:37:VAL:HA	0.54	2.03	19	9
1:B:38:ILE:HD12	1:B:69:THR:CG2	0.54	2.32	18	2
1:A:54:LEU:HD23	1:A:70:GLN:NE2	0.54	2.17	12	1
1:B:96:ALA:O	1:B:100:PHE:N	0.54	2.40	14	16
1:B:40:LEU:HD23	1:B:67:MET:N	0.54	2.17	16	8
1:A:10:LYS:HG3	1:A:79:ILE:O	0.54	2.02	13	1
1:A:26:SER:O	1:A:30:ASP:CA	0.54	2.56	13	13
1:B:2:SER:O	1:B:30:ASP:HB2	0.54	2.02	4	5
1:B:75:VAL:HG23	1:B:75:VAL:O	0.54	2.00	5	5
1:A:24:VAL:HG11	1:A:38:ILE:HG12	0.54	1.79	18	1
1:B:38:ILE:HG23	1:B:67:MET:HE2	0.54	1.79	2	1
1:B:43:ILE:HD12	1:B:57:THR:HG22	0.54	1.78	17	2
1:B:26:SER:O	1:B:30:ASP:CA	0.54	2.56	6	9
1:B:10:LYS:CG	1:B:79:ILE:O	0.54	2.55	6	2
1:A:35:ARG:HH21	1:A:77:VAL:HG23	0.54	1.61	17	1
1:A:7:TYR:CE1	1:A:23:ASP:HB2	0.54	2.37	4	7
1:B:20:TYR:OH	1:B:65:PHE:CZ	0.54	2.61	8	10
1:B:20:TYR:HB2	1:B:40:LEU:HD12	0.54	1.79	12	3
1:A:87:LEU:HD12	1:A:87:LEU:N	0.54	2.18	8	11
1:B:69:THR:HG22	1:B:101:LEU:CD1	0.54	2.31	6	2
1:B:36:LEU:HD21	1:B:72:MET:HG2	0.54	1.79	7	1
1:B:6:LEU:HD12	1:B:60:ILE:HD13	0.54	1.80	11	1
1:B:60:ILE:HD11	1:B:62:GLU:HB2	0.54	1.80	11	2
1:A:40:LEU:HD21	1:A:58:ILE:CG2	0.54	2.32	19	1
1:A:102:ILE:HG21	1:B:102:ILE:HG21	0.54	1.79	8	5
1:B:29:LEU:HA	1:B:32:LEU:HD23	0.54	1.79	1	1
1:B:40:LEU:HD22	1:B:58:ILE:HD12	0.54	1.80	5	2
1:A:98:ILE:HG23	1:A:102:ILE:CG1	0.54	2.33	6	2
1:B:101:LEU:HD22	1:B:101:LEU:O	0.54	2.03	13	3
1:B:10:LYS:HG2	1:B:79:ILE:HD11	0.54	1.79	7	1
1:A:58:ILE:CD1	1:A:59:HIS:N	0.54	2.67	10	2
1:B:58:ILE:CD1	1:B:60:ILE:N	0.54	2.71	1	1
1:B:58:ILE:HG22	1:B:90:PHE:CG	0.54	2.37	6	3
1:B:22:VAL:HG11	1:B:94:ILE:HD12	0.54	1.79	18	2
1:B:67:MET:HE1	1:B:93:GLU:C	0.54	2.27	18	1
1:A:15:ALA:HA	1:A:19:PRO:CA	0.53	2.33	8	18
1:B:7:TYR:CE1	1:B:23:ASP:HB2	0.53	2.38	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:8:LYS:CA	1:B:19:PRO:O	0.53	2.56	1	1
1:B:15:ALA:HA	1:B:19:PRO:CA	0.53	2.33	17	17
1:B:33:ASN:C	1:B:34:THR:HG22	0.53	2.28	13	7
1:B:7:TYR:HB2	1:B:81:SER:OG	0.53	2.03	7	8
1:B:37:VAL:CG2	1:B:73:THR:HG23	0.53	2.33	4	1
1:B:58:ILE:CG2	1:B:59:HIS:N	0.53	2.71	13	3
1:B:9:ASN:CB	1:B:14:SER:HB3	0.53	2.33	8	3
1:A:28:LEU:O	1:A:32:LEU:HD13	0.53	2.03	17	3
1:B:6:LEU:CG	1:B:87:LEU:HG	0.53	2.33	15	3
1:B:26:SER:HB2	1:B:35:ARG:CD	0.53	2.33	14	1
1:A:68:LEU:HD22	1:A:70:GLN:CG	0.53	2.33	5	1
1:B:58:ILE:HD13	1:B:58:ILE:H	0.53	1.63	8	5
1:A:24:VAL:HB	1:A:94:ILE:CG2	0.53	2.32	7	6
1:A:56:PRO:HG2	1:A:67:MET:HE3	0.53	1.78	20	1
1:A:15:ALA:HA	1:A:18:TYR:C	0.53	2.28	16	20
1:B:7:TYR:HB3	1:B:81:SER:CB	0.53	2.33	2	9
1:A:7:TYR:CB	1:A:81:SER:OG	0.53	2.56	15	8
1:A:9:ASN:C	1:A:11:ASP:N	0.53	2.65	12	11
1:B:40:LEU:HD21	1:B:67:MET:HG3	0.53	1.79	3	1
1:A:42:PRO:HG3	1:A:45:LEU:HD23	0.53	1.78	4	1
1:B:42:PRO:N	1:B:65:PHE:CD2	0.53	2.76	6	3
1:A:89:THR:HG23	1:A:90:PHE:HD1	0.53	1.61	7	1
1:B:17:THR:HG23	1:B:18:TYR:N	0.53	2.18	13	1
1:A:101:LEU:HD22	1:A:101:LEU:O	0.53	2.03	15	1
1:A:25:GLN:HB2	1:A:36:LEU:HB3	0.53	1.80	6	9
1:B:9:ASN:C	1:B:11:ASP:N	0.53	2.66	4	18
1:B:15:ALA:HA	1:B:19:PRO:N	0.53	2.19	17	12
1:B:38:ILE:HD12	1:B:97:ALA:HB1	0.53	1.80	2	1
1:A:79:ILE:CG1	1:A:79:ILE:O	0.53	2.56	11	3
1:B:54:LEU:O	1:B:69:THR:HG21	0.53	2.03	8	1
1:B:35:ARG:CZ	1:B:80:LEU:HD13	0.53	2.32	17	1
1:A:8:LYS:HA	1:A:19:PRO:O	0.53	2.04	5	6
1:A:41:THR:O	1:A:65:PHE:HB3	0.53	2.04	13	8
1:B:24:VAL:O	1:B:25:GLN:HB2	0.53	2.03	15	8
1:B:68:LEU:HD23	1:B:71:GLN:CB	0.53	2.33	5	3
1:A:7:TYR:CB	1:A:81:SER:HB3	0.53	2.33	6	3
1:B:24:VAL:HA	1:B:35:ARG:NH1	0.53	2.19	10	1
1:A:38:ILE:HD12	1:A:94:ILE:HG23	0.53	1.80	11	3
1:B:58:ILE:HG12	1:B:87:LEU:HD12	0.53	1.81	13	1
1:A:8:LYS:CA	1:A:20:TYR:HB3	0.53	2.29	16	1
1:B:10:LYS:CA	1:B:82:GLU:H	0.53	2.17	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:CG2	1:A:90:PHE:CE2	0.53	2.91	17	2
1:B:4:PHE:HZ	1:B:95:ILE:HD11	0.53	1.64	11	1
1:B:40:LEU:CD2	1:B:67:MET:HE3	0.53	2.33	14	1
1:A:56:PRO:HD2	1:A:67:MET:HB2	0.53	1.81	16	4
1:B:2:SER:OG	1:B:31:ASN:HB2	0.53	2.04	4	2
1:A:10:LYS:HB2	1:A:79:ILE:HG12	0.53	1.79	5	1
1:A:29:LEU:HD13	1:B:70:GLN:HG2	0.53	1.81	10	1
1:A:35:ARG:CD	1:A:80:LEU:HD11	0.53	2.34	12	1
1:A:60:ILE:CD1	1:A:87:LEU:HD23	0.53	2.24	15	1
1:A:24:VAL:O	1:A:25:GLN:HB2	0.53	2.03	4	10
1:B:87:LEU:HD12	1:B:87:LEU:N	0.53	2.17	3	12
1:B:101:LEU:HG	1:B:102:ILE:N	0.53	2.19	8	9
1:A:2:SER:O	1:A:3:GLN:HB3	0.53	2.03	5	2
1:A:7:TYR:HB3	1:A:81:SER:HB3	0.53	1.80	8	1
1:B:9:ASN:HD21	1:B:12:LYS:HA	0.53	1.64	14	3
1:A:72:MET:HB3	1:B:36:LEU:HD21	0.53	1.81	17	1
1:A:2:SER:HB3	1:A:30:ASP:HB3	0.53	1.81	20	1
1:A:10:LYS:C	1:A:10:LYS:CD	0.53	2.82	1	2
1:B:58:ILE:HB	1:B:90:PHE:CE2	0.53	2.38	1	2
1:A:23:ASP:HA	1:A:37:VAL:HG12	0.53	1.80	18	6
1:A:7:TYR:CE1	1:A:23:ASP:CB	0.53	2.91	19	5
1:A:35:ARG:CG	1:A:37:VAL:HG13	0.53	2.33	1	1
1:A:24:VAL:CG2	1:A:98:ILE:HD13	0.53	2.34	12	6
1:A:56:PRO:HD2	1:A:67:MET:CB	0.53	2.34	13	2
1:A:102:ILE:HD12	1:A:102:ILE:C	0.53	2.29	16	2
1:A:68:LEU:HD23	1:A:71:GLN:HB2	0.53	1.81	20	1
1:A:98:ILE:HG22	1:A:99:ASP:N	0.52	2.19	20	7
1:B:38:ILE:CG2	1:B:67:MET:HB3	0.52	2.34	11	5
1:A:98:ILE:HG23	1:A:102:ILE:HG12	0.52	1.81	11	4
1:B:9:ASN:OD1	1:B:12:LYS:HA	0.52	2.04	5	5
1:B:40:LEU:HD22	1:B:58:ILE:CD1	0.52	2.34	15	2
1:B:2:SER:OG	1:B:31:ASN:HB3	0.52	2.04	19	2
1:B:26:SER:O	1:B:30:ASP:N	0.52	2.42	13	8
1:B:36:LEU:CD2	1:B:72:MET:HE3	0.52	2.26	16	2
1:B:39:PRO:O	1:B:68:LEU:CB	0.52	2.57	15	4
1:B:2:SER:HB3	1:B:30:ASP:OD2	0.52	2.04	6	1
1:B:102:ILE:HD12	1:B:102:ILE:C	0.52	2.29	10	2
1:B:24:VAL:HG21	1:B:38:ILE:HD12	0.52	1.82	15	1
1:B:20:TYR:HB2	1:B:40:LEU:CD1	0.52	2.34	2	2
1:A:35:ARG:CD	1:A:37:VAL:HG13	0.52	2.33	8	1
1:A:101:LEU:HD23	1:A:102:ILE:CG2	0.52	2.34	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASP:OD2	1:A:80:LEU:HD11	0.52	2.04	15	1
1:A:36:LEU:HG	1:A:72:MET:HE3	0.52	1.80	15	1
1:A:84:VAL:HG22	1:A:85:ASN:OD1	0.52	2.05	16	1
1:A:22:VAL:HG21	1:A:67:MET:HE2	0.52	1.80	17	1
1:B:92:ASN:O	1:B:95:ILE:N	0.52	2.43	18	17
1:A:81:SER:O	1:A:83:PRO:HD3	0.52	2.04	12	3
1:A:7:TYR:HB2	1:A:81:SER:OG	0.52	2.05	15	9
1:A:8:LYS:HB3	1:A:82:GLU:O	0.52	2.05	7	3
1:A:30:ASP:O	1:A:35:ARG:CG	0.52	2.58	20	4
1:B:17:THR:HG22	1:B:18:TYR:CE1	0.52	2.40	11	5
1:A:21:PHE:CE2	1:A:81:SER:OG	0.52	2.60	6	1
1:B:101:LEU:CD1	1:B:102:ILE:CG1	0.52	2.88	13	3
1:B:7:TYR:C	1:B:81:SER:CB	0.52	2.82	2	6
1:A:58:ILE:HD12	1:A:87:LEU:CD1	0.52	2.34	14	2
1:A:9:ASN:CG	1:A:21:PHE:CZ	0.52	2.87	5	2
1:B:38:ILE:HB	1:B:67:MET:HE2	0.52	1.82	5	4
1:A:43:ILE:HG12	1:A:57:THR:HG22	0.52	1.82	7	2
1:A:10:LYS:HD2	1:A:79:ILE:HG13	0.52	1.80	10	1
1:B:64:ASP:O	1:B:65:PHE:HD1	0.52	1.88	15	1
1:A:54:LEU:HD21	1:A:100:PHE:CE2	0.52	2.40	6	1
1:B:9:ASN:ND2	1:B:12:LYS:HA	0.52	2.20	6	4
1:A:22:VAL:CG1	1:A:94:ILE:CG1	0.52	2.88	18	1
1:B:100:PHE:CB	1:B:105:ILE:HG22	0.52	2.34	19	1
1:B:10:LYS:HD2	1:B:79:ILE:CG1	0.52	2.35	2	6
1:B:8:LYS:N	1:B:81:SER:HB3	0.52	2.19	2	1
1:B:37:VAL:HG21	1:B:75:VAL:HG13	0.52	1.81	11	2
1:A:38:ILE:N	1:A:38:ILE:HD12	0.52	2.19	6	1
1:A:72:MET:HE2	1:A:102:ILE:HD11	0.52	1.82	8	1
1:B:38:ILE:HG23	1:B:69:THR:HB	0.52	1.81	12	1
1:B:54:LEU:HD23	1:B:55:CYS:SG	0.52	2.43	12	1
1:B:43:ILE:HG23	1:B:48:LYS:CD	0.52	2.35	17	1
1:A:35:ARG:NE	1:A:80:LEU:HD23	0.52	2.19	20	1
1:A:15:ALA:HA	1:A:19:PRO:N	0.52	2.20	4	16
1:A:33:ASN:C	1:A:34:THR:HG22	0.52	2.30	5	10
1:A:101:LEU:HG	1:A:102:ILE:N	0.52	2.20	9	7
1:A:38:ILE:CG2	1:A:67:MET:HB3	0.52	2.35	14	6
1:A:26:SER:HB2	1:A:29:LEU:HB2	0.52	1.82	6	1
1:B:43:ILE:HB	1:B:66:ILE:HG13	0.52	1.80	17	1
1:A:35:ARG:NH2	1:A:80:LEU:HD13	0.52	2.20	1	1
1:B:6:LEU:HD21	1:B:40:LEU:HD13	0.52	1.82	1	2
1:B:33:ASN:C	1:B:34:THR:CG2	0.52	2.83	11	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:LEU:N	1:B:28:LEU:CD1	0.52	2.73	19	6
1:A:8:LYS:HB2	1:A:84:VAL:CG1	0.52	2.35	8	4
1:B:20:TYR:C	1:B:21:PHE:CD1	0.52	2.88	7	12
1:B:38:ILE:HD11	1:B:94:ILE:HG23	0.52	1.81	3	1
1:A:58:ILE:HG23	1:A:60:ILE:HG23	0.52	1.82	5	2
1:B:6:LEU:HD13	1:B:87:LEU:CD2	0.52	2.34	6	2
1:B:58:ILE:CG2	1:B:90:PHE:CE2	0.52	2.90	7	3
1:A:2:SER:OG	1:A:31:ASN:HB2	0.52	2.05	9	1
1:A:75:VAL:HG11	1:A:79:ILE:HD13	0.52	1.81	11	1
1:B:8:LYS:HB3	1:B:82:GLU:O	0.52	2.04	13	1
1:A:36:LEU:HD22	1:B:72:MET:CE	0.52	2.35	14	1
1:A:41:THR:O	1:A:66:ILE:CD1	0.51	2.58	16	8
1:A:98:ILE:O	1:A:102:ILE:N	0.51	2.41	8	13
1:B:20:TYR:OH	1:B:65:PHE:CE2	0.51	2.60	5	7
1:B:7:TYR:CD2	1:B:80:LEU:CD1	0.51	2.93	7	5
1:B:99:ASP:O	1:B:103:THR:HB	0.51	2.04	13	9
1:A:36:LEU:HD21	1:B:72:MET:CE	0.51	2.35	6	1
1:B:33:ASN:O	1:B:77:VAL:HG12	0.51	2.05	20	1
1:A:54:LEU:HD21	1:A:69:THR:CG2	0.51	2.35	2	1
1:B:17:THR:HG22	1:B:18:TYR:CZ	0.51	2.40	2	3
1:B:24:VAL:HB	1:B:94:ILE:CG2	0.51	2.35	14	8
1:A:7:TYR:CB	1:A:81:SER:CB	0.51	2.88	13	6
1:A:36:LEU:HD21	1:A:72:MET:CE	0.51	2.33	17	1
1:A:58:ILE:HD13	1:A:90:PHE:CD1	0.51	2.40	17	1
1:B:26:SER:O	1:B:30:ASP:HB2	0.51	2.05	17	3
1:B:24:VAL:O	1:B:25:GLN:CB	0.51	2.59	10	7
1:B:10:LYS:NZ	1:B:79:ILE:HD11	0.51	2.20	5	1
1:B:25:GLN:HB2	1:B:36:LEU:CB	0.51	2.35	6	4
1:A:22:VAL:O	1:A:37:VAL:HA	0.51	2.05	17	3
1:B:8:LYS:O	1:B:81:SER:CB	0.51	2.59	13	1
1:B:58:ILE:CD1	1:B:60:ILE:H	0.51	2.17	1	1
1:A:10:LYS:N	1:A:82:GLU:N	0.51	2.59	8	2
1:A:72:MET:SD	1:B:72:MET:HE1	0.51	2.46	4	1
1:B:25:GLN:CG	1:B:36:LEU:HB2	0.51	2.35	6	3
1:B:2:SER:CB	1:B:31:ASN:HB3	0.51	2.36	13	4
1:A:7:TYR:CE2	1:A:23:ASP:OD2	0.51	2.64	9	5
1:A:7:TYR:HB3	1:A:81:SER:CB	0.51	2.36	8	8
1:A:76:PRO:CD	1:A:79:ILE:HD11	0.51	2.35	15	3
1:A:7:TYR:CE2	1:A:80:LEU:CD2	0.51	2.94	17	1
1:B:24:VAL:HG22	1:B:98:ILE:CD1	0.51	2.36	1	5
1:B:58:ILE:HA	1:B:90:PHE:CE2	0.51	2.41	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:VAL:HG23	1:B:79:ILE:HG23	0.51	1.82	17	3
1:B:24:VAL:HG12	1:B:94:ILE:HG23	0.51	1.82	17	2
1:B:67:MET:HE1	1:B:97:ALA:HB2	0.51	1.82	20	1
1:A:8:LYS:CA	1:A:19:PRO:O	0.51	2.59	5	6
1:A:9:ASN:H	1:A:20:TYR:HA	0.51	1.66	18	4
1:A:20:TYR:OH	1:A:65:PHE:CD2	0.51	2.63	13	4
1:B:99:ASP:HB3	1:B:105:ILE:HD11	0.51	1.82	1	1
1:A:7:TYR:CZ	1:A:23:ASP:OD2	0.51	2.64	12	6
1:B:38:ILE:HD12	1:B:67:MET:SD	0.51	2.46	5	3
1:A:8:LYS:C	1:A:81:SER:HB3	0.51	2.30	12	3
1:A:69:THR:HG22	1:A:101:LEU:CD2	0.51	2.24	4	1
1:A:28:LEU:N	1:A:28:LEU:CD1	0.51	2.74	9	7
1:B:6:LEU:HD13	1:B:87:LEU:CG	0.51	2.35	6	1
1:A:70:GLN:OE1	1:B:29:LEU:HD13	0.51	2.05	14	1
1:B:43:ILE:CG2	1:B:66:ILE:HG23	0.51	2.35	15	1
1:B:35:ARG:CD	1:B:37:VAL:HG13	0.51	2.34	17	1
1:B:5:THR:CB	1:B:7:TYR:CZ	0.51	2.94	20	16
1:A:72:MET:CE	1:A:102:ILE:HD11	0.51	2.35	12	4
1:A:67:MET:HE1	1:A:94:ILE:HA	0.51	1.81	11	2
1:A:72:MET:HE1	1:A:98:ILE:CD1	0.51	2.35	15	2
1:A:10:LYS:CD	1:A:79:ILE:CG1	0.51	2.89	12	6
1:B:27:ASP:CG	1:B:28:LEU:HD22	0.51	2.31	6	1
1:B:29:LEU:O	1:B:34:THR:O	0.51	2.29	10	1
1:B:7:TYR:CZ	1:B:23:ASP:HB2	0.51	2.41	14	2
1:A:101:LEU:CD1	1:A:102:ILE:CG1	0.51	2.89	15	1
1:A:35:ARG:NH2	1:A:80:LEU:HA	0.51	2.19	18	1
1:A:34:THR:C	1:A:35:ARG:HG2	0.51	2.31	20	1
1:A:35:ARG:CZ	1:A:37:VAL:HG11	0.51	2.36	1	1
1:B:8:LYS:HG3	1:B:19:PRO:O	0.51	2.05	12	12
1:B:8:LYS:C	1:B:81:SER:OG	0.51	2.54	11	2
1:B:54:LEU:HD23	1:B:101:LEU:HD13	0.51	1.83	4	1
1:B:101:LEU:HD22	1:B:102:ILE:N	0.51	2.21	6	3
1:B:54:LEU:HD23	1:B:55:CYS:N	0.51	2.21	12	1
1:A:7:TYR:OH	1:A:35:ARG:NH1	0.51	2.44	13	1
1:A:33:ASN:C	1:A:34:THR:CG2	0.50	2.84	12	12
1:A:95:ILE:O	1:A:96:ALA:C	0.50	2.54	14	15
1:A:98:ILE:HA	1:A:102:ILE:HG13	0.50	1.83	14	11
1:A:7:TYR:CE1	1:A:23:ASP:CG	0.50	2.89	14	5
1:B:7:TYR:N	1:B:7:TYR:CD1	0.50	2.79	2	3
1:B:38:ILE:HD12	1:B:97:ALA:CB	0.50	2.36	2	1
1:B:10:LYS:CD	1:B:79:ILE:CG1	0.50	2.89	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:GLN:HG3	1:B:36:LEU:CB	0.50	2.36	9	5
1:A:105:ILE:HD12	1:A:105:ILE:C	0.50	2.31	1	1
1:B:34:THR:HG22	1:B:76:PRO:HA	0.50	1.82	4	3
1:A:34:THR:HA	1:A:77:VAL:HG13	0.50	1.83	9	1
1:A:62:GLU:OE2	1:A:84:VAL:HG22	0.50	2.06	9	1
1:A:23:ASP:CG	1:A:80:LEU:HD21	0.50	2.31	15	1
1:B:31:ASN:ND2	1:B:77:VAL:HG23	0.50	2.20	18	1
1:A:43:ILE:HD11	1:A:57:THR:HG23	0.50	1.80	19	1
1:A:8:LYS:N	1:A:81:SER:HB3	0.50	2.22	12	6
1:A:24:VAL:HG22	1:A:98:ILE:CD1	0.50	2.36	4	4
1:A:40:LEU:HD23	1:A:67:MET:HG2	0.50	1.84	2	1
1:B:10:LYS:HG3	1:B:79:ILE:HG12	0.50	1.83	2	5
1:B:38:ILE:CD1	1:B:69:THR:HB	0.50	2.36	2	1
1:A:22:VAL:CG2	1:A:67:MET:HE3	0.50	2.36	4	1
1:B:38:ILE:HD11	1:B:94:ILE:O	0.50	2.06	5	1
1:A:97:ALA:O	1:A:101:LEU:HB2	0.50	2.06	19	2
1:A:101:LEU:CD2	1:A:101:LEU:O	0.50	2.59	15	1
1:A:36:LEU:HD22	1:B:72:MET:HE2	0.50	1.82	16	1
1:B:7:TYR:CB	1:B:81:SER:OG	0.50	2.60	17	11
1:A:8:LYS:O	1:A:9:ASN:O	0.50	2.30	16	5
1:B:64:ASP:C	1:B:65:PHE:CD1	0.50	2.89	5	5
1:B:35:ARG:HG2	1:B:36:LEU:N	0.50	2.22	3	1
1:B:6:LEU:H	1:B:86:GLU:HA	0.50	1.66	19	3
1:B:41:THR:O	1:B:65:PHE:HB3	0.50	2.07	5	6
1:A:54:LEU:HD21	1:A:101:LEU:HB2	0.50	1.84	13	1
1:A:56:PRO:CG	1:A:67:MET:HE3	0.50	2.37	20	1
1:B:67:MET:HE1	1:B:94:ILE:CD1	0.50	2.37	2	1
1:A:38:ILE:CD1	1:A:67:MET:CB	0.50	2.90	7	1
1:B:98:ILE:HA	1:B:101:LEU:HD13	0.50	1.84	13	2
1:A:35:ARG:HG3	1:A:37:VAL:HG13	0.50	1.83	1	1
1:B:3:GLN:O	1:B:23:ASP:O	0.50	2.29	3	2
1:B:38:ILE:HD13	1:B:67:MET:CB	0.50	2.37	2	1
1:B:10:LYS:HG2	1:B:79:ILE:CA	0.50	2.37	5	1
1:B:41:THR:O	1:B:66:ILE:N	0.50	2.44	9	5
1:B:79:ILE:O	1:B:79:ILE:HG12	0.50	2.05	7	1
1:A:75:VAL:HG23	1:A:79:ILE:HG23	0.50	1.83	8	2
1:A:56:PRO:CG	1:A:67:MET:HE2	0.50	2.37	11	1
1:A:60:ILE:HD11	1:A:65:PHE:CE2	0.50	2.42	12	1
1:A:6:LEU:HD13	1:A:87:LEU:HD21	0.50	1.84	17	1
1:A:2:SER:HB2	1:A:31:ASN:HB3	0.50	1.84	18	1
1:A:5:THR:O	1:A:7:TYR:CD1	0.50	2.65	5	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:SER:HB3	1:B:29:LEU:HB2	0.50	1.83	5	12
1:A:6:LEU:CD2	1:A:20:TYR:CD2	0.50	2.95	16	4
1:A:23:ASP:CG	1:A:35:ARG:HD2	0.50	2.32	9	1
1:A:6:LEU:HD13	1:A:87:LEU:HD13	0.49	1.82	1	1
1:A:35:ARG:NH2	1:A:75:VAL:HG21	0.49	2.21	1	1
1:A:24:VAL:HG11	1:A:94:ILE:CG2	0.49	2.37	11	4
1:B:40:LEU:CD2	1:B:67:MET:HG2	0.49	2.36	2	3
1:A:20:TYR:OH	1:A:65:PHE:CD1	0.49	2.65	7	7
1:A:35:ARG:HD2	1:A:37:VAL:HG13	0.49	1.84	8	1
1:B:42:PRO:HG2	1:B:45:LEU:HD12	0.49	1.83	19	3
1:A:105:ILE:OXT	1:A:105:ILE:HG22	0.49	2.07	13	1
1:B:29:LEU:O	1:B:35:ARG:NH2	0.49	2.46	18	2
1:B:7:TYR:CZ	1:B:23:ASP:OD2	0.49	2.65	19	10
1:B:7:TYR:CB	1:B:81:SER:CB	0.49	2.89	11	9
1:A:2:SER:CB	1:A:30:ASP:C	0.49	2.85	9	5
1:B:2:SER:HB3	1:B:30:ASP:HB2	0.49	1.83	4	2
1:A:30:ASP:OD2	1:A:35:ARG:CZ	0.49	2.60	5	1
1:B:37:VAL:CG2	1:B:75:VAL:HG13	0.49	2.37	5	2
1:B:38:ILE:HG23	1:B:69:THR:CB	0.49	2.36	7	1
1:B:8:LYS:O	1:B:8:LYS:HD2	0.49	2.08	11	1
1:A:35:ARG:HD2	1:A:75:VAL:O	0.49	2.07	18	1
1:B:31:ASN:CG	1:B:31:ASN:O	0.49	2.55	6	2
1:A:2:SER:O	1:A:3:GLN:CG	0.49	2.60	20	2
1:A:54:LEU:HD21	1:A:69:THR:HB	0.49	1.83	5	1
1:A:43:ILE:HG23	1:A:48:LYS:HG2	0.49	1.83	6	1
1:A:71:GLN:O	1:A:72:MET:O	0.49	2.30	11	5
1:A:38:ILE:HD13	1:A:67:MET:CB	0.49	2.36	7	1
1:B:3:GLN:HB2	1:B:35:ARG:NH1	0.49	2.23	11	1
1:B:9:ASN:ND2	1:B:9:ASN:O	0.49	2.42	12	1
1:B:60:ILE:HD11	1:B:65:PHE:HD2	0.49	1.67	12	1
1:A:99:ASP:O	1:A:105:ILE:CD1	0.49	2.60	14	1
1:A:40:LEU:HD11	1:A:67:MET:HE3	0.49	1.84	15	1
1:A:30:ASP:HA	1:A:35:ARG:CD	0.49	2.37	15	2
1:B:35:ARG:HB3	1:B:35:ARG:CZ	0.49	2.38	17	2
1:A:22:VAL:CG2	1:A:40:LEU:HD11	0.49	2.37	4	1
1:A:22:VAL:HG11	1:A:94:ILE:HD12	0.49	1.83	13	2
1:A:72:MET:CE	1:B:36:LEU:HD21	0.49	2.37	5	1
1:A:43:ILE:CG2	1:A:48:LYS:CD	0.49	2.90	6	1
1:B:101:LEU:CD2	1:B:101:LEU:O	0.49	2.60	14	3
1:A:8:LYS:CD	1:A:20:TYR:CD2	0.49	2.95	15	2
1:B:54:LEU:HD11	1:B:101:LEU:HD13	0.49	1.84	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LYS:HG2	1:A:79:ILE:HB	0.49	1.85	15	2
1:B:24:VAL:HG21	1:B:38:ILE:HD11	0.49	1.82	15	1
1:B:7:TYR:CZ	1:B:23:ASP:CG	0.49	2.91	5	10
1:B:8:LYS:N	1:B:81:SER:HB2	0.49	2.22	20	6
1:A:38:ILE:HG23	1:A:38:ILE:O	0.49	2.08	7	1
1:A:24:VAL:N	1:A:35:ARG:NH1	0.49	2.61	10	1
1:A:60:ILE:HG22	1:A:61:ASP:N	0.49	2.23	15	1
1:A:3:GLN:O	1:A:4:PHE:CG	0.49	2.66	16	1
1:B:98:ILE:O	1:B:102:ILE:N	0.49	2.41	5	7
1:A:92:ASN:O	1:A:93:GLU:C	0.49	2.56	20	14
1:B:41:THR:O	1:B:66:ILE:CD1	0.49	2.61	9	11
1:A:94:ILE:N	1:A:94:ILE:HD13	0.49	2.23	13	2
1:B:10:LYS:HE2	1:B:79:ILE:HG12	0.49	1.82	5	1
1:B:58:ILE:HD12	1:B:87:LEU:CD1	0.49	2.36	7	1
1:A:35:ARG:HD3	1:A:36:LEU:H	0.49	1.68	3	1
1:B:23:ASP:CA	1:B:35:ARG:HD2	0.49	2.36	3	1
1:B:9:ASN:N	1:B:81:SER:CB	0.49	2.76	5	3
1:A:38:ILE:HD11	1:A:69:THR:OG1	0.49	2.07	7	1
1:B:20:TYR:CD1	1:B:40:LEU:HD12	0.49	2.42	15	1
1:A:38:ILE:HG23	1:A:69:THR:CA	0.49	2.38	18	2
1:A:10:LYS:HG2	1:A:79:ILE:HG13	0.49	1.84	18	1
1:B:95:ILE:O	1:B:96:ALA:C	0.49	2.56	19	9
1:A:8:LYS:C	1:A:20:TYR:HA	0.49	2.32	3	2
1:A:6:LEU:HB2	1:A:87:LEU:HD13	0.49	1.84	4	1
1:B:6:LEU:C	1:B:6:LEU:HD23	0.49	2.33	9	2
1:B:54:LEU:HD11	1:B:101:LEU:CA	0.49	2.38	9	1
1:B:7:TYR:CB	1:B:81:SER:HB3	0.49	2.37	16	5
1:A:43:ILE:HD11	1:A:57:THR:HG1	0.49	1.67	20	2
1:A:58:ILE:HD11	1:A:67:MET:SD	0.49	2.48	17	1
1:A:35:ARG:CD	1:A:35:ARG:O	0.49	2.61	18	1
1:B:5:THR:O	1:B:7:TYR:CD1	0.49	2.66	10	16
1:B:30:ASP:O	1:B:35:ARG:CG	0.49	2.60	9	4
1:B:10:LYS:HA	1:B:82:GLU:CB	0.49	2.38	2	1
1:B:23:ASP:C	1:B:35:ARG:NH1	0.49	2.71	12	1
1:A:98:ILE:HA	1:A:101:LEU:HD13	0.49	1.83	15	1
1:B:99:ASP:HB3	1:B:105:ILE:HG21	0.49	1.84	19	1
1:A:58:ILE:HG23	1:A:90:PHE:CZ	0.49	2.42	3	4
1:A:8:LYS:HB2	1:A:84:VAL:HB	0.49	1.82	3	3
1:B:58:ILE:HG23	1:B:90:PHE:CG	0.49	2.43	15	2
1:B:92:ASN:O	1:B:93:GLU:C	0.49	2.56	3	13
1:B:71:GLN:O	1:B:72:MET:O	0.49	2.30	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:THR:HG23	1:A:86:GLU:CG	0.49	2.37	8	1
1:B:72:MET:CE	1:B:98:ILE:HD11	0.49	2.33	12	2
1:B:17:THR:CG2	1:B:18:TYR:N	0.49	2.76	13	1
1:B:38:ILE:CG1	1:B:69:THR:HG23	0.49	2.38	18	1
1:A:98:ILE:CA	1:A:101:LEU:HD23	0.48	2.38	3	4
1:B:10:LYS:N	1:B:82:GLU:N	0.48	2.60	1	1
1:A:26:SER:HB2	1:A:35:ARG:CZ	0.48	2.38	3	2
1:B:99:ASP:O	1:B:103:THR:OG1	0.48	2.30	17	4
1:A:66:ILE:HD12	1:A:66:ILE:N	0.48	2.23	17	6
1:B:54:LEU:HD21	1:B:101:LEU:HB2	0.48	1.85	5	3
1:A:25:GLN:HG3	1:A:36:LEU:CB	0.48	2.37	14	5
1:B:8:LYS:HG3	1:B:9:ASN:OD1	0.48	2.08	7	1
1:B:41:THR:OG1	1:B:46:LEU:HD22	0.48	2.08	18	2
1:B:58:ILE:HD13	1:B:90:PHE:CG	0.48	2.43	18	2
1:A:72:MET:O	1:A:73:THR:HG23	0.48	2.08	16	1
1:B:6:LEU:HD21	1:B:60:ILE:CD1	0.48	2.33	19	1
1:B:98:ILE:CA	1:B:101:LEU:HD23	0.48	2.38	2	2
1:A:7:TYR:CD1	1:A:7:TYR:N	0.48	2.81	15	8
1:B:20:TYR:O	1:B:21:PHE:CD1	0.48	2.66	7	7
1:B:21:PHE:HA	1:B:38:ILE:O	0.48	2.08	4	1
1:B:8:LYS:CB	1:B:84:VAL:HB	0.48	2.38	7	1
1:B:98:ILE:CG2	1:B:102:ILE:HD11	0.48	2.39	10	2
1:A:40:LEU:HD23	1:A:67:MET:N	0.48	2.23	18	5
1:A:75:VAL:HG22	1:A:79:ILE:CD1	0.48	2.38	13	1
1:B:40:LEU:HD11	1:B:67:MET:HE3	0.48	1.85	14	1
1:A:8:LYS:CG	1:A:19:PRO:O	0.48	2.61	1	8
1:A:64:ASP:C	1:A:65:PHE:CD1	0.48	2.91	1	4
1:B:42:PRO:HG3	1:B:45:LEU:HD12	0.48	1.83	6	8
1:A:58:ILE:HG23	1:A:90:PHE:CG	0.48	2.43	9	3
1:A:58:ILE:HG23	1:A:59:HIS:N	0.48	2.23	5	3
1:A:23:ASP:HB3	1:A:35:ARG:HD3	0.48	1.85	7	1
1:A:43:ILE:HD11	1:A:66:ILE:HG23	0.48	1.82	8	1
1:B:30:ASP:HA	1:B:35:ARG:HD2	0.48	1.86	14	1
1:A:38:ILE:CG2	1:A:69:THR:HB	0.48	2.38	3	2
1:B:36:LEU:HD12	1:B:73:THR:O	0.48	2.08	3	1
1:B:58:ILE:CG1	1:B:90:PHE:CD2	0.48	2.96	4	3
1:B:2:SER:HB2	1:B:31:ASN:HB2	0.48	1.84	5	1
1:B:26:SER:O	1:B:35:ARG:NH1	0.48	2.47	15	1
1:A:42:PRO:N	1:A:65:PHE:CD2	0.48	2.82	16	1
1:B:2:SER:CB	1:B:31:ASN:CB	0.48	2.91	6	4
1:B:26:SER:O	1:B:30:ASP:HB3	0.48	2.07	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:66:ILE:HD12	1:B:66:ILE:N	0.48	2.23	7	6
1:A:35:ARG:HB3	1:A:35:ARG:CZ	0.48	2.39	8	1
1:A:38:ILE:HG12	1:A:38:ILE:O	0.48	2.09	12	1
1:B:57:THR:HG23	1:B:58:ILE:N	0.48	2.23	12	2
1:B:75:VAL:HG13	1:B:80:LEU:HD22	0.48	1.85	12	1
1:A:23:ASP:HA	1:A:35:ARG:HG3	0.48	1.85	16	1
1:B:26:SER:O	1:B:30:ASP:CB	0.48	2.62	16	1
1:B:22:VAL:HG12	1:B:94:ILE:HG21	0.48	1.84	18	1
1:B:23:ASP:OD2	1:B:35:ARG:NE	0.48	2.47	19	1
1:A:99:ASP:OD1	1:A:105:ILE:HD11	0.48	2.07	5	1
1:B:60:ILE:HD11	1:B:87:LEU:HD23	0.48	1.84	15	1
1:A:6:LEU:HG	1:A:87:LEU:HG	0.48	1.86	16	1
1:B:21:PHE:CD2	1:B:75:VAL:HG11	0.48	2.44	11	2
1:B:79:ILE:O	1:B:80:LEU:O	0.48	2.32	6	1
1:A:23:ASP:CA	1:A:35:ARG:HD2	0.48	2.39	11	1
1:A:10:LYS:HB2	1:A:79:ILE:CG1	0.48	2.39	1	1
1:B:7:TYR:HB3	1:B:81:SER:HB2	0.48	1.86	2	4
1:A:10:LYS:HB3	1:A:79:ILE:CB	0.48	2.39	2	6
1:A:58:ILE:HD13	1:A:90:PHE:CE2	0.48	2.44	3	1
1:B:8:LYS:HB3	1:B:84:VAL:HB	0.48	1.86	12	4
1:A:58:ILE:CD1	1:A:60:ILE:H	0.48	2.21	10	2
1:B:57:THR:HA	1:B:66:ILE:CG2	0.48	2.39	11	1
1:B:8:LYS:CD	1:B:20:TYR:CD2	0.48	2.96	13	1
1:A:31:ASN:ND2	1:A:80:LEU:HD21	0.48	2.24	3	1
1:B:23:ASP:CB	1:B:35:ARG:HD3	0.48	2.39	3	1
1:A:101:LEU:CD1	1:A:102:ILE:HG23	0.48	2.39	6	2
1:B:40:LEU:HG	1:B:67:MET:HG2	0.48	1.85	7	3
1:B:2:SER:O	1:B:3:GLN:HB2	0.48	2.08	17	2
1:B:24:VAL:HG11	1:B:38:ILE:HD12	0.48	1.85	12	1
1:B:24:VAL:HG22	1:B:36:LEU:O	0.48	2.09	20	2
1:B:19:PRO:HG2	1:B:41:THR:HA	0.47	1.85	6	5
1:B:102:ILE:CG1	1:B:103:THR:HG23	0.47	2.38	15	3
1:A:38:ILE:HD12	1:A:67:MET:SD	0.47	2.49	3	1
1:B:37:VAL:HG22	1:B:73:THR:C	0.47	2.34	4	1
1:B:60:ILE:HD12	1:B:85:ASN:ND2	0.47	2.24	11	1
1:A:69:THR:HB	1:A:101:LEU:HD22	0.47	1.86	12	3
1:A:58:ILE:HG21	1:A:87:LEU:CD1	0.47	2.28	14	1
1:A:39:PRO:O	1:A:68:LEU:CB	0.47	2.61	17	9
1:A:15:ALA:CB	1:A:19:PRO:HB3	0.47	2.39	8	7
1:B:43:ILE:HD11	1:B:57:THR:HG22	0.47	1.84	3	1
1:A:54:LEU:C	1:A:54:LEU:HD22	0.47	2.34	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:TYR:CE1	1:B:23:ASP:CB	0.47	2.98	4	1
1:A:38:ILE:HG21	1:A:67:MET:HB3	0.47	1.85	19	2
1:B:35:ARG:NH1	1:B:80:LEU:HD23	0.47	2.24	6	1
1:B:60:ILE:HG22	1:B:61:ASP:N	0.47	2.25	15	1
1:A:6:LEU:HD22	1:A:87:LEU:HG	0.47	1.86	17	1
1:A:2:SER:O	1:A:30:ASP:CB	0.47	2.62	3	2
1:B:22:VAL:HG21	1:B:67:MET:CE	0.47	2.34	2	2
1:A:98:ILE:O	1:A:102:ILE:HG13	0.47	2.10	16	3
1:B:58:ILE:CA	1:B:90:PHE:CZ	0.47	2.97	6	1
1:A:25:GLN:CB	1:A:36:LEU:HB3	0.47	2.40	11	2
1:B:25:GLN:OE1	1:B:36:LEU:HD22	0.47	2.09	11	1
1:B:40:LEU:CD1	1:B:67:MET:HE3	0.47	2.39	14	1
1:A:46:LEU:HD22	1:A:66:ILE:HD13	0.47	1.86	18	1
1:A:38:ILE:HG23	1:A:69:THR:HA	0.47	1.85	16	6
1:B:9:ASN:C	1:B:81:SER:HA	0.47	2.33	3	2
1:B:2:SER:CB	1:B:31:ASN:HB2	0.47	2.40	5	4
1:B:29:LEU:HA	1:B:32:LEU:HD13	0.47	1.84	9	2
1:A:44:GLU:HA	1:A:48:LYS:HG2	0.47	1.86	8	2
1:A:35:ARG:HD3	1:A:37:VAL:HG13	0.47	1.86	18	1
1:B:99:ASP:O	1:B:104:GLY:N	0.47	2.47	10	7
1:B:35:ARG:HG3	1:B:36:LEU:N	0.47	2.24	2	2
1:A:58:ILE:HD12	1:A:87:LEU:HD12	0.47	1.86	4	1
1:B:82:GLU:O	1:B:84:VAL:N	0.47	2.47	7	3
1:A:2:SER:CB	1:A:31:ASN:HB2	0.47	2.39	9	3
1:A:103:THR:HG22	1:B:103:THR:CG2	0.47	2.40	10	1
1:B:99:ASP:CB	1:B:105:ILE:HD12	0.47	2.39	10	1
1:B:101:LEU:CD1	1:B:102:ILE:HG23	0.47	2.39	10	2
1:B:24:VAL:HG13	1:B:98:ILE:HD11	0.47	1.85	11	1
1:B:41:THR:HG21	1:B:68:LEU:HD22	0.47	1.85	12	1
1:B:58:ILE:CG2	1:B:90:PHE:CG	0.47	2.98	15	1
1:A:72:MET:CB	1:B:36:LEU:HD21	0.47	2.39	17	1
1:B:41:THR:CG2	1:B:68:LEU:HD13	0.47	2.38	19	1
1:B:2:SER:CB	1:B:30:ASP:C	0.47	2.88	3	5
1:B:10:LYS:HG2	1:B:79:ILE:CG1	0.47	2.39	7	2
1:A:41:THR:HG21	1:A:68:LEU:HD22	0.47	1.87	18	2
1:B:7:TYR:CD1	1:B:7:TYR:N	0.47	2.82	12	6
1:B:35:ARG:CD	1:B:80:LEU:CD1	0.47	2.92	1	1
1:A:88:SER:O	1:A:91:ARG:HG2	0.47	2.10	14	13
1:B:26:SER:HB2	1:B:35:ARG:CZ	0.47	2.39	18	3
1:B:94:ILE:N	1:B:94:ILE:HD12	0.47	2.25	14	4
1:A:22:VAL:CG1	1:A:94:ILE:CG2	0.47	2.93	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:94:ILE:HD13	1:B:94:ILE:N	0.47	2.25	3	1
1:B:58:ILE:HG13	1:B:90:PHE:CE1	0.47	2.44	13	3
1:B:22:VAL:CG1	1:B:94:ILE:CG1	0.47	2.87	6	3
1:A:2:SER:HB2	1:A:31:ASN:HB2	0.47	1.85	7	2
1:A:25:GLN:HE21	1:B:72:MET:HE1	0.47	1.70	7	1
1:A:8:LYS:C	1:A:81:SER:OG	0.47	2.57	9	1
1:A:29:LEU:HD22	1:B:70:GLN:HE21	0.47	1.69	9	1
1:A:59:HIS:CE1	1:A:90:PHE:CZ	0.47	3.03	10	1
1:B:10:LYS:O	1:B:82:GLU:HB2	0.47	2.10	16	3
1:A:70:GLN:HG2	1:B:29:LEU:HD13	0.47	1.87	12	1
1:A:54:LEU:O	1:A:56:PRO:HD3	0.47	2.10	13	1
1:A:98:ILE:HG12	1:A:102:ILE:HD12	0.47	1.86	13	1
1:B:97:ALA:O	1:B:101:LEU:N	0.47	2.43	13	2
1:A:19:PRO:HG2	1:A:20:TYR:CE1	0.47	2.45	14	2
1:A:35:ARG:CZ	1:A:35:ARG:HA	0.47	2.38	15	1
1:A:35:ARG:NE	1:A:36:LEU:H	0.47	2.06	15	1
1:B:54:LEU:HD21	1:B:101:LEU:HD13	0.47	1.86	18	1
1:A:80:LEU:C	1:A:80:LEU:HD12	0.47	2.35	19	1
1:B:98:ILE:O	1:B:102:ILE:HB	0.47	2.10	1	7
1:B:98:ILE:HG23	1:B:102:ILE:HD12	0.47	1.87	3	3
1:A:8:LYS:N	1:A:81:SER:OG	0.47	2.48	8	2
1:A:36:LEU:HD21	1:A:72:MET:SD	0.47	2.50	7	1
1:A:58:ILE:HG22	1:A:90:PHE:CD2	0.47	2.45	11	1
1:B:43:ILE:HG12	1:B:48:LYS:CD	0.47	2.40	14	5
1:B:21:PHE:N	1:B:21:PHE:CD1	0.47	2.83	12	1
1:B:80:LEU:HD12	1:B:80:LEU:O	0.47	2.10	12	1
1:A:24:VAL:HG11	1:A:38:ILE:HD12	0.47	1.85	14	1
1:B:24:VAL:HG11	1:B:94:ILE:HG23	0.47	1.84	15	1
1:B:8:LYS:HB2	1:B:84:VAL:CG1	0.47	2.40	1	7
1:B:88:SER:O	1:B:91:ARG:HG2	0.47	2.10	11	15
1:A:24:VAL:N	1:A:35:ARG:HD2	0.47	2.25	5	1
1:A:79:ILE:O	1:A:80:LEU:O	0.47	2.32	6	1
1:A:36:LEU:HD11	1:A:72:MET:SD	0.47	2.50	8	1
1:B:40:LEU:HD23	1:B:67:MET:SD	0.47	2.50	9	1
1:B:94:ILE:CD1	1:B:94:ILE:N	0.47	2.77	20	2
1:B:101:LEU:HG	1:B:102:ILE:HG23	0.47	1.85	10	2
1:A:60:ILE:HD11	1:A:65:PHE:CD2	0.47	2.45	14	1
1:A:40:LEU:HD21	1:A:58:ILE:HG23	0.47	1.85	19	1
1:A:2:SER:HB2	1:A:30:ASP:CG	0.47	2.35	1	1
1:A:21:PHE:CG	1:A:75:VAL:HG11	0.47	2.44	5	1
1:A:58:ILE:HG22	1:A:90:PHE:CD1	0.47	2.44	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:TYR:C	1:A:21:PHE:CD1	0.46	2.93	17	11
1:B:2:SER:HB2	1:B:31:ASN:HB3	0.46	1.86	13	3
1:B:35:ARG:CD	1:B:80:LEU:HD11	0.46	2.40	1	1
1:B:43:ILE:HD12	1:B:64:ASP:HB2	0.46	1.87	1	1
1:A:7:TYR:CB	1:A:81:SER:HB2	0.46	2.40	2	5
1:A:19:PRO:CG	1:A:42:PRO:CD	0.46	2.92	2	2
1:B:23:ASP:HA	1:B:35:ARG:HD2	0.46	1.86	3	1
1:A:10:LYS:CD	1:A:79:ILE:HG13	0.46	2.41	4	3
1:A:17:THR:HG22	1:A:18:TYR:CZ	0.46	2.45	16	3
1:B:59:HIS:N	1:B:90:PHE:CZ	0.46	2.84	15	1
1:A:20:TYR:CG	1:A:40:LEU:HD13	0.46	2.44	16	1
1:B:38:ILE:HG23	1:B:72:MET:HE2	0.46	1.87	19	1
1:B:2:SER:O	1:B:3:GLN:HB3	0.46	2.10	20	1
1:A:41:THR:O	1:A:66:ILE:N	0.46	2.48	18	6
1:A:26:SER:O	1:A:30:ASP:HB2	0.46	2.10	20	3
1:B:43:ILE:HD11	1:B:66:ILE:HG23	0.46	1.86	3	1
1:B:37:VAL:HG23	1:B:73:THR:HG23	0.46	1.87	4	1
1:A:28:LEU:O	1:A:32:LEU:HD21	0.46	2.11	5	1
1:B:4:PHE:CE2	1:B:91:ARG:HB2	0.46	2.46	11	6
1:A:67:MET:SD	1:A:94:ILE:HD12	0.46	2.50	20	2
1:A:9:ASN:ND2	1:A:21:PHE:CZ	0.46	2.84	7	2
1:B:6:LEU:HD22	1:B:84:VAL:CG1	0.46	2.39	8	3
1:B:3:GLN:CB	1:B:35:ARG:NH2	0.46	2.78	15	1
1:B:58:ILE:HD12	1:B:59:HIS:CA	0.46	2.39	1	1
1:A:40:LEU:HA	1:A:67:MET:HA	0.46	1.87	16	2
1:B:87:LEU:O	1:B:87:LEU:CG	0.46	2.63	5	3
1:A:10:LYS:HD2	1:A:79:ILE:HG12	0.46	1.85	12	5
1:B:8:LYS:C	1:B:81:SER:HB2	0.46	2.35	6	2
1:A:42:PRO:HG2	1:A:45:LEU:HD12	0.46	1.86	8	3
1:A:35:ARG:HG3	1:A:80:LEU:HD11	0.46	1.87	12	1
1:A:57:THR:HG22	1:A:58:ILE:N	0.46	2.24	19	2
1:A:6:LEU:HD13	1:A:87:LEU:CD2	0.46	2.41	17	1
1:B:7:TYR:CB	1:B:81:SER:HB2	0.46	2.40	11	4
1:B:10:LYS:CA	1:B:82:GLU:N	0.46	2.78	9	4
1:B:23:ASP:HB3	1:B:35:ARG:CD	0.46	2.40	8	2
1:B:57:THR:HG22	1:B:58:ILE:N	0.46	2.25	8	3
1:B:102:ILE:CD1	1:B:102:ILE:C	0.46	2.88	11	2
1:A:72:MET:HE1	1:A:102:ILE:HD13	0.46	1.87	1	1
1:B:10:LYS:CD	1:B:79:ILE:HG12	0.46	2.41	1	1
1:B:20:TYR:C	1:B:40:LEU:HD12	0.46	2.36	6	2
1:B:69:THR:HB	1:B:101:LEU:HD22	0.46	1.88	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLU:CG	1:A:48:LYS:HG3	0.46	2.40	6	1
1:B:10:LYS:HG2	1:B:79:ILE:HB	0.46	1.87	6	1
1:B:4:PHE:CE1	1:B:95:ILE:HD11	0.46	2.45	14	1
1:B:90:PHE:O	1:B:94:ILE:HD13	0.46	2.11	16	1
1:B:35:ARG:NH1	1:B:80:LEU:HD13	0.46	2.26	17	1
1:A:10:LYS:HB3	1:A:79:ILE:HG22	0.46	1.88	7	5
1:A:9:ASN:C	1:A:81:SER:HA	0.46	2.36	10	3
1:A:95:ILE:O	1:A:99:ASP:N	0.46	2.46	16	3
1:B:101:LEU:CD2	1:B:102:ILE:HG12	0.46	2.41	13	3
1:A:8:LYS:C	1:A:81:SER:HB2	0.46	2.36	20	2
1:B:6:LEU:CD2	1:B:20:TYR:CD2	0.46	2.99	17	4
1:A:30:ASP:O	1:A:35:ARG:CD	0.46	2.64	13	2
1:A:6:LEU:N	1:A:87:LEU:HD22	0.46	2.26	20	2
1:A:2:SER:CB	1:A:31:ASN:HB3	0.46	2.40	20	2
1:A:7:TYR:CD2	1:A:80:LEU:HD22	0.46	2.46	16	1
1:B:15:ALA:CB	1:B:19:PRO:HB3	0.46	2.41	4	3
1:B:98:ILE:HA	1:B:102:ILE:HG13	0.46	1.88	4	13
1:B:21:PHE:CB	1:B:37:VAL:HB	0.46	2.40	4	14
1:B:25:GLN:HG2	1:B:36:LEU:HD23	0.46	1.87	2	1
1:A:6:LEU:CD1	1:A:40:LEU:HD13	0.46	2.40	4	1
1:A:40:LEU:CD2	1:A:58:ILE:CD1	0.46	2.94	9	1
1:B:41:THR:OG1	1:B:42:PRO:CD	0.46	2.62	20	9
1:A:101:LEU:HD12	1:B:25:GLN:HE22	0.46	1.70	5	1
1:A:25:GLN:NE2	1:B:101:LEU:CD2	0.46	2.79	6	2
1:A:99:ASP:O	1:A:103:THR:HB	0.46	2.11	12	4
1:B:43:ILE:HD11	1:B:48:LYS:HG3	0.46	1.86	20	3
1:A:75:VAL:HG22	1:A:79:ILE:HD11	0.46	1.86	13	1
1:A:40:LEU:HD22	1:A:65:PHE:CB	0.46	2.41	19	1
1:A:10:LYS:HA	1:A:81:SER:CA	0.46	2.39	1	1
1:A:94:ILE:HD12	1:A:94:ILE:N	0.46	2.26	7	5
1:B:75:VAL:HG21	1:B:79:ILE:O	0.46	2.11	12	3
1:A:98:ILE:CA	1:A:102:ILE:HG23	0.46	2.41	3	2
1:A:23:ASP:N	1:A:37:VAL:HG12	0.46	2.26	5	7
1:B:58:ILE:HG23	1:B:59:HIS:N	0.46	2.26	16	3
1:B:6:LEU:O	1:B:6:LEU:HD23	0.46	2.11	5	1
1:A:58:ILE:HD13	1:A:65:PHE:O	0.46	2.10	7	1
1:B:30:ASP:HA	1:B:35:ARG:CG	0.46	2.41	7	1
1:A:7:TYR:O	1:A:21:PHE:N	0.46	2.46	8	1
1:B:64:ASP:C	1:B:65:PHE:CD2	0.46	2.94	8	1
1:A:23:ASP:HB3	1:A:35:ARG:CD	0.46	2.41	13	1
1:A:101:LEU:CD2	1:A:102:ILE:HG12	0.46	2.40	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:TYR:CZ	1:A:23:ASP:CB	0.46	2.99	17	2
1:B:35:ARG:NE	1:B:35:ARG:CA	0.46	2.77	20	2
1:B:38:ILE:CD1	1:B:67:MET:CB	0.46	2.94	2	1
1:A:9:ASN:ND2	1:A:15:ALA:N	0.46	2.64	3	1
1:A:10:LYS:CD	1:A:79:ILE:HG12	0.46	2.41	12	4
1:A:10:LYS:HG2	1:A:79:ILE:CA	0.46	2.41	13	1
1:A:8:LYS:CB	1:A:84:VAL:HG13	0.46	2.41	15	1
1:A:35:ARG:HG3	1:A:80:LEU:CD2	0.46	2.40	20	1
1:B:98:ILE:O	1:B:102:ILE:HG23	0.45	2.11	17	3
1:A:58:ILE:HG23	1:A:67:MET:HE1	0.45	1.88	6	1
1:B:72:MET:HE1	1:B:98:ILE:CG1	0.45	2.40	10	1
1:B:71:GLN:OE1	1:B:73:THR:HG23	0.45	2.11	11	1
1:A:35:ARG:NE	1:A:80:LEU:HD13	0.45	2.25	14	1
1:A:22:VAL:HG11	1:A:94:ILE:HD11	0.45	1.87	18	1
1:B:57:THR:OG1	1:B:66:ILE:CG2	0.45	2.64	1	2
1:A:40:LEU:CA	1:A:67:MET:HA	0.45	2.41	16	2
1:A:98:ILE:O	1:A:102:ILE:HG23	0.45	2.11	3	2
1:B:6:LEU:HB2	1:B:87:LEU:HG	0.45	1.88	6	3
1:B:75:VAL:CG2	1:B:80:LEU:HD22	0.45	2.42	4	1
1:A:40:LEU:HD21	1:A:67:MET:CG	0.45	2.41	7	1
1:B:25:GLN:HG2	1:B:26:SER:N	0.45	2.25	11	2
1:A:38:ILE:HD11	1:A:98:ILE:CD1	0.45	2.41	20	1
1:A:77:VAL:HG13	1:A:78:LYS:N	0.45	2.27	5	12
1:B:6:LEU:HD13	1:B:84:VAL:CG1	0.45	2.41	1	1
1:B:58:ILE:HG23	1:B:90:PHE:CZ	0.45	2.47	7	4
1:A:37:VAL:CG2	1:A:75:VAL:HG13	0.45	2.41	4	1
1:A:60:ILE:HD11	1:A:62:GLU:HB2	0.45	1.87	4	1
1:A:98:ILE:CG2	1:A:102:ILE:HG12	0.45	2.41	11	2
1:B:10:LYS:C	1:B:82:GLU:HB2	0.45	2.36	9	5
1:A:8:LYS:O	1:A:81:SER:HB2	0.45	2.10	8	2
1:B:20:TYR:CE1	1:B:65:PHE:CD2	0.45	3.05	9	1
1:B:41:THR:HG23	1:B:66:ILE:HD11	0.45	1.85	15	1
1:A:6:LEU:HB2	1:A:87:LEU:HD22	0.45	1.87	1	1
1:A:9:ASN:HA	1:A:21:PHE:CZ	0.45	2.47	1	1
1:B:77:VAL:HG13	1:B:78:LYS:N	0.45	2.27	9	13
1:A:22:VAL:HG12	1:A:94:ILE:HG21	0.45	1.87	3	2
1:A:9:ASN:ND2	1:A:21:PHE:CE2	0.45	2.84	5	1
1:A:2:SER:CB	1:A:30:ASP:HB2	0.45	2.41	7	3
1:B:24:VAL:O	1:B:36:LEU:HD12	0.45	2.12	7	1
1:A:23:ASP:CB	1:A:35:ARG:NH1	0.45	2.80	13	1
1:A:10:LYS:HD2	1:A:11:ASP:H	0.45	1.71	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PHE:CB	1:A:37:VAL:HB	0.45	2.42	9	16
1:B:2:SER:HB2	1:B:31:ASN:CA	0.45	2.41	9	2
1:A:35:ARG:HD3	1:A:36:LEU:N	0.45	2.26	11	1
1:B:9:ASN:ND2	1:B:21:PHE:CZ	0.45	2.85	18	2
1:A:35:ARG:NE	1:A:80:LEU:CD1	0.45	2.79	14	1
1:B:43:ILE:HD11	1:B:48:LYS:HD2	0.45	1.87	14	1
1:A:65:PHE:CD1	1:A:65:PHE:N	0.45	2.85	16	1
1:B:38:ILE:HG23	1:B:69:THR:HA	0.45	1.88	15	4
1:B:24:VAL:HB	1:B:94:ILE:HG22	0.45	1.88	18	2
1:A:30:ASP:O	1:A:35:ARG:HG3	0.45	2.12	5	1
1:B:6:LEU:HD21	1:B:20:TYR:CD2	0.45	2.46	9	3
1:A:10:LYS:O	1:A:82:GLU:HB2	0.45	2.12	18	3
1:B:22:VAL:CG1	1:B:94:ILE:HG13	0.45	2.40	7	3
1:B:37:VAL:CG2	1:B:73:THR:O	0.45	2.63	7	1
1:A:38:ILE:CG2	1:A:69:THR:CG2	0.45	2.95	12	2
1:B:40:LEU:HD23	1:B:67:MET:HE2	0.45	1.89	9	1
1:B:72:MET:HE1	1:B:98:ILE:HG12	0.45	1.89	10	1
1:B:87:LEU:CD2	1:B:87:LEU:H	0.45	2.25	16	1
1:B:35:ARG:HB2	1:B:35:ARG:NH1	0.45	2.27	19	1
1:A:38:ILE:HD11	1:A:94:ILE:HA	0.45	1.87	1	1
1:B:9:ASN:CA	1:B:81:SER:HA	0.45	2.41	1	1
1:B:10:LYS:HD2	1:B:79:ILE:HG12	0.45	1.89	1	1
1:B:67:MET:HE1	1:B:94:ILE:HG12	0.45	1.88	1	1
1:A:35:ARG:HG3	1:A:36:LEU:N	0.45	2.26	2	1
1:A:33:ASN:C	1:A:34:THR:HG23	0.45	2.37	4	6
1:B:55:CYS:O	1:B:66:ILE:HG22	0.45	2.12	3	1
1:A:10:LYS:CA	1:A:82:GLU:N	0.45	2.79	10	5
1:A:36:LEU:HD11	1:B:72:MET:HE2	0.45	1.87	4	1
1:A:25:GLN:HE21	1:A:36:LEU:HD22	0.45	1.72	5	2
1:B:69:THR:HG22	1:B:72:MET:HE1	0.45	1.88	5	2
1:A:55:CYS:CB	1:A:67:MET:O	0.45	2.65	6	2
1:A:35:ARG:HD2	1:A:80:LEU:CD2	0.45	2.42	9	1
1:B:58:ILE:N	1:B:58:ILE:CD1	0.45	2.80	12	1
1:A:58:ILE:HB	1:A:90:PHE:CE2	0.45	2.47	11	5
1:B:17:THR:HG22	1:B:18:TYR:CE2	0.45	2.46	2	1
1:B:33:ASN:C	1:B:34:THR:HG23	0.45	2.37	12	8
1:A:2:SER:O	1:A:35:ARG:NH1	0.45	2.50	4	1
1:A:21:PHE:CD1	1:A:21:PHE:N	0.45	2.84	4	1
1:A:90:PHE:O	1:A:94:ILE:HD13	0.45	2.12	6	3
1:B:35:ARG:NH2	1:B:77:VAL:HB	0.45	2.27	5	1
1:A:9:ASN:CB	1:A:14:SER:HB3	0.45	2.41	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ASP:O	1:A:104:GLY:N	0.45	2.49	13	2
1:A:101:LEU:HD22	1:A:102:ILE:N	0.45	2.25	15	1
1:B:21:PHE:CD1	1:B:21:PHE:N	0.45	2.84	15	1
1:B:58:ILE:CD1	1:B:90:PHE:CD2	0.45	2.99	17	1
1:A:64:ASP:C	1:A:65:PHE:CG	0.45	2.94	17	11
1:B:54:LEU:CG	1:B:69:THR:HG23	0.45	2.42	2	1
1:B:23:ASP:CB	1:B:35:ARG:CD	0.45	2.95	3	1
1:B:76:PRO:O	1:B:77:VAL:C	0.45	2.60	14	9
1:A:10:LYS:C	1:A:82:GLU:HB2	0.45	2.37	10	6
1:A:8:LYS:HG2	1:A:19:PRO:O	0.45	2.10	5	1
1:A:7:TYR:CE1	1:A:23:ASP:HB3	0.45	2.47	19	2
1:B:25:GLN:NE2	1:B:26:SER:CB	0.45	2.80	8	1
1:B:8:LYS:O	1:B:81:SER:CA	0.45	2.65	11	1
1:B:30:ASP:CB	1:B:35:ARG:NE	0.45	2.80	11	1
1:B:57:THR:HA	1:B:66:ILE:HG23	0.45	1.87	11	1
1:B:7:TYR:CE2	1:B:80:LEU:CD2	0.45	3.00	15	1
1:A:11:ASP:O	1:A:13:SER:N	0.45	2.50	19	1
1:A:88:SER:O	1:A:91:ARG:CD	0.45	2.65	16	8
1:B:7:TYR:HB3	1:B:81:SER:OG	0.45	2.12	1	1
1:B:99:ASP:CB	1:B:105:ILE:HD11	0.45	2.42	1	1
1:A:57:THR:OG1	1:A:65:PHE:O	0.45	2.31	2	2
1:B:98:ILE:CA	1:B:102:ILE:HG23	0.45	2.42	2	3
1:A:20:TYR:O	1:A:21:PHE:CD1	0.45	2.70	3	4
1:A:97:ALA:C	1:A:101:LEU:HD23	0.45	2.36	6	2
1:B:87:LEU:HB2	1:B:90:PHE:HB2	0.45	1.89	14	3
1:A:25:GLN:NE2	1:B:101:LEU:CD1	0.45	2.80	19	2
1:A:38:ILE:HG12	1:A:69:THR:HG23	0.45	1.88	13	1
1:A:24:VAL:O	1:A:24:VAL:HG13	0.45	2.11	16	1
1:A:6:LEU:CG	1:A:87:LEU:HD13	0.45	2.42	18	1
1:B:2:SER:O	1:B:35:ARG:HD2	0.45	2.12	19	1
1:A:19:PRO:HG2	1:A:41:THR:HA	0.44	1.89	5	3
1:B:17:THR:CG2	1:B:18:TYR:CE2	0.44	3.00	15	2
1:B:24:VAL:CG2	1:B:98:ILE:CD1	0.44	2.95	3	9
1:A:10:LYS:N	1:A:82:GLU:H	0.44	2.09	12	5
1:B:19:PRO:HG2	1:B:42:PRO:HD3	0.44	1.88	9	5
1:B:57:THR:HG1	1:B:66:ILE:HG23	0.44	1.71	9	3
1:B:6:LEU:HD23	1:B:6:LEU:C	0.44	2.37	5	1
1:B:7:TYR:HB3	1:B:81:SER:O	0.44	2.12	5	1
1:A:25:GLN:NE2	1:B:101:LEU:HD23	0.44	2.27	6	1
1:A:2:SER:O	1:A:3:GLN:HB2	0.44	2.11	8	2
1:B:10:LYS:CA	1:B:81:SER:HA	0.44	2.42	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:VAL:O	1:B:36:LEU:HB3	0.44	2.12	7	1
1:B:8:LYS:CG	1:B:19:PRO:O	0.44	2.65	16	4
1:B:95:ILE:O	1:B:99:ASP:N	0.44	2.47	11	2
1:A:6:LEU:H	1:A:86:GLU:HA	0.44	1.72	13	1
1:A:69:THR:HG22	1:A:72:MET:HE3	0.44	1.89	14	1
1:B:43:ILE:CG2	1:B:66:ILE:CG2	0.44	2.95	15	1
1:B:25:GLN:O	1:B:26:SER:C	0.44	2.61	9	3
1:A:9:ASN:CB	1:A:14:SER:HB2	0.44	2.42	18	4
1:A:35:ARG:NE	1:A:35:ARG:CA	0.44	2.74	3	2
1:A:43:ILE:CD1	1:A:57:THR:OG1	0.44	2.65	14	4
1:A:98:ILE:O	1:A:102:ILE:CB	0.44	2.64	20	2
1:B:5:THR:O	1:B:7:TYR:CE1	0.44	2.70	2	7
1:B:98:ILE:HG23	1:B:102:ILE:HG12	0.44	1.88	10	2
1:A:29:LEU:O	1:A:35:ARG:NH2	0.44	2.50	3	1
1:A:9:ASN:OD1	1:A:21:PHE:CE1	0.44	2.70	14	2
1:A:102:ILE:HG12	1:B:102:ILE:HG21	0.44	1.89	6	1
1:B:99:ASP:HA	1:B:103:THR:HB	0.44	1.88	6	1
1:A:2:SER:O	1:A:30:ASP:CG	0.44	2.60	20	2
1:A:4:PHE:CD2	1:A:91:ARG:HB3	0.44	2.48	14	1
1:B:105:ILE:HD12	1:B:105:ILE:O	0.44	2.13	17	1
1:A:95:ILE:O	1:A:98:ILE:N	0.44	2.51	2	1
1:B:36:LEU:HG	1:B:72:MET:HE3	0.44	1.89	2	1
1:B:45:LEU:C	1:B:45:LEU:CD1	0.44	2.89	2	1
1:B:23:ASP:HB3	1:B:35:ARG:HD3	0.44	1.90	3	2
1:B:7:TYR:CE1	1:B:23:ASP:HB3	0.44	2.47	4	1
1:A:58:ILE:CG1	1:A:90:PHE:CD2	0.44	3.00	20	2
1:A:43:ILE:HD12	1:A:64:ASP:C	0.44	2.37	7	1
1:B:69:THR:CG2	1:B:101:LEU:CD2	0.44	2.95	7	2
1:B:98:ILE:O	1:B:102:ILE:HG13	0.44	2.12	10	3
1:A:29:LEU:O	1:A:35:ARG:NH1	0.44	2.50	15	1
1:A:10:LYS:HB3	1:A:79:ILE:CG1	0.44	2.39	18	1
1:A:24:VAL:CB	1:A:94:ILE:HG23	0.44	2.42	18	1
1:A:41:THR:OG1	1:A:42:PRO:CD	0.44	2.66	3	4
1:B:8:LYS:HB2	1:B:20:TYR:CD2	0.44	2.48	9	6
1:B:58:ILE:CG1	1:B:90:PHE:CE2	0.44	3.00	4	1
1:A:9:ASN:HB2	1:A:14:SER:HB3	0.44	1.88	5	1
1:A:21:PHE:HB2	1:A:37:VAL:HB	0.44	1.90	5	1
1:B:9:ASN:OD1	1:B:15:ALA:HB2	0.44	2.12	6	1
1:A:56:PRO:C	1:A:66:ILE:HG22	0.44	2.37	7	1
1:B:38:ILE:HG21	1:B:67:MET:SD	0.44	2.52	12	1
1:B:8:LYS:HB2	1:B:84:VAL:HB	0.44	1.89	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LYS:CD	1:A:20:TYR:CE2	0.44	3.00	15	1
1:A:31:ASN:HB2	1:A:35:ARG:CZ	0.44	2.43	17	1
1:B:24:VAL:HG11	1:B:38:ILE:HD13	0.44	1.87	17	1
1:B:24:VAL:CB	1:B:94:ILE:HG22	0.44	2.42	18	1
1:B:15:ALA:HB1	1:B:19:PRO:HB3	0.44	1.89	4	3
1:B:22:VAL:CG1	1:B:94:ILE:CG2	0.44	2.95	1	5
1:B:19:PRO:HD2	1:B:40:LEU:O	0.44	2.13	5	3
1:A:6:LEU:HD21	1:A:20:TYR:CD2	0.44	2.47	16	4
1:A:102:ILE:CD1	1:A:102:ILE:C	0.44	2.91	6	1
1:A:75:VAL:O	1:A:80:LEU:HD22	0.44	2.12	10	1
1:B:2:SER:O	1:B:30:ASP:CB	0.44	2.66	10	2
1:B:10:LYS:O	1:B:82:GLU:CB	0.44	2.65	11	1
1:B:31:ASN:CG	1:B:80:LEU:HD12	0.44	2.36	14	2
1:A:4:PHE:CD2	1:A:91:ARG:CB	0.44	3.00	14	2
1:B:87:LEU:CD2	1:B:87:LEU:N	0.44	2.80	16	1
1:A:4:PHE:CD1	1:A:4:PHE:N	0.44	2.84	18	1
1:B:3:GLN:N	1:B:7:TYR:OH	0.44	2.46	2	1
1:B:26:SER:HB2	1:B:35:ARG:NE	0.44	2.27	20	2
1:B:81:SER:O	1:B:83:PRO:HD3	0.44	2.13	2	2
1:A:31:ASN:ND2	1:A:80:LEU:CD2	0.44	2.81	3	2
1:A:33:ASN:O	1:A:77:VAL:HG12	0.44	2.12	3	1
1:B:35:ARG:C	1:B:35:ARG:NE	0.44	2.76	3	1
1:B:58:ILE:HG13	1:B:90:PHE:CZ	0.44	2.47	4	1
1:B:58:ILE:HA	1:B:90:PHE:CE1	0.44	2.46	6	1
1:B:6:LEU:HD12	1:B:87:LEU:HG	0.44	1.90	8	1
1:A:103:THR:CG2	1:B:103:THR:HG22	0.44	2.43	10	1
1:A:102:ILE:C	1:A:102:ILE:CD1	0.44	2.90	16	1
1:B:10:LYS:HA	1:B:82:GLU:H	0.44	1.72	18	3
1:B:6:LEU:HD23	1:B:85:ASN:CB	0.44	2.41	19	2
1:B:101:LEU:HG	1:B:102:ILE:CG1	0.44	2.43	8	5
1:B:21:PHE:CD2	1:B:81:SER:OG	0.44	2.71	5	2
1:B:58:ILE:CD1	1:B:67:MET:HE1	0.44	2.42	14	1
1:B:20:TYR:CE1	1:B:65:PHE:HD2	0.44	2.30	15	1
1:A:6:LEU:HD22	1:A:84:VAL:CG1	0.44	2.42	19	1
1:A:101:LEU:HD23	1:A:102:ILE:CG1	0.44	2.42	20	1
1:A:42:PRO:HG3	1:A:45:LEU:HD12	0.44	1.89	1	8
1:A:60:ILE:HD12	1:A:62:GLU:HB2	0.44	1.90	2	2
1:A:30:ASP:HA	1:A:35:ARG:NE	0.44	2.27	3	1
1:B:35:ARG:HB3	1:B:35:ARG:NH1	0.44	2.28	3	2
1:B:24:VAL:CG1	1:B:38:ILE:CG1	0.44	2.96	4	1
1:B:24:VAL:HG11	1:B:94:ILE:HG22	0.44	1.90	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD22	1:A:85:ASN:HB3	0.44	1.90	5	1
1:A:24:VAL:HG13	1:A:98:ILE:HD11	0.44	1.90	8	3
1:B:98:ILE:HA	1:B:102:ILE:CD1	0.44	2.42	14	2
1:B:41:THR:HG21	1:B:68:LEU:HD12	0.44	1.90	18	1
1:A:58:ILE:CD1	1:A:67:MET:HE2	0.44	2.42	20	1
1:A:54:LEU:HD22	1:B:29:LEU:CD1	0.44	2.43	1	1
1:A:15:ALA:HB1	1:A:19:PRO:HB3	0.44	1.89	3	5
1:A:77:VAL:HA	1:A:80:LEU:HD23	0.44	1.90	3	1
1:B:40:LEU:CD2	1:B:58:ILE:CD1	0.44	2.96	3	1
1:A:87:LEU:HD22	1:A:87:LEU:H	0.44	1.73	4	1
1:B:44:GLU:HA	1:B:48:LYS:HG2	0.44	1.90	10	2
1:A:40:LEU:CD2	1:A:58:ILE:HD11	0.44	2.43	9	1
1:A:3:GLN:O	1:A:23:ASP:O	0.44	2.36	10	2
1:B:38:ILE:CG2	1:B:69:THR:CG2	0.44	2.95	19	2
1:A:31:ASN:O	1:A:32:LEU:C	0.44	2.60	12	1
1:A:3:GLN:N	1:A:35:ARG:NH1	0.44	2.65	13	1
1:B:8:LYS:HD2	1:B:20:TYR:CD2	0.44	2.48	13	1
1:A:42:PRO:CA	1:A:65:PHE:CD2	0.44	3.00	16	1
1:B:54:LEU:HD21	1:B:69:THR:HB	0.44	1.89	16	1
1:B:38:ILE:HD12	1:B:72:MET:HE2	0.44	1.89	19	1
1:B:20:TYR:OH	1:B:65:PHE:CD2	0.43	2.68	6	2
1:A:25:GLN:CD	1:A:26:SER:N	0.43	2.77	4	1
1:A:30:ASP:HA	1:A:35:ARG:HG2	0.43	1.90	4	1
1:B:3:GLN:HA	1:B:23:ASP:HB2	0.43	1.90	16	1
1:A:10:LYS:CB	1:A:79:ILE:CG1	0.43	2.95	18	1
1:A:46:LEU:HD21	1:A:68:LEU:HD11	0.43	1.90	18	1
1:A:58:ILE:HD11	1:A:67:MET:HG3	0.43	1.90	2	1
1:A:87:LEU:CD2	1:A:87:LEU:H	0.43	2.27	18	2
1:B:96:ALA:O	1:B:100:PHE:HB3	0.43	2.12	4	3
1:A:101:LEU:HG	1:A:102:ILE:CG1	0.43	2.44	7	3
1:B:20:TYR:OH	1:B:60:ILE:HD11	0.43	2.13	6	1
1:A:102:ILE:HD13	1:B:102:ILE:HG21	0.43	1.90	7	1
1:A:34:THR:HG21	1:B:71:GLN:OE1	0.43	2.13	8	1
1:A:26:SER:O	1:A:30:ASP:CG	0.43	2.61	13	2
1:B:80:LEU:C	1:B:81:SER:OG	0.43	2.62	9	1
1:A:69:THR:CG2	1:A:101:LEU:HD13	0.43	2.44	10	1
1:B:38:ILE:CG2	1:B:69:THR:HB	0.43	2.43	12	1
1:B:72:MET:HE1	1:B:98:ILE:CD1	0.43	2.35	12	1
1:A:6:LEU:HB2	1:A:87:LEU:HG	0.43	1.89	15	2
1:B:46:LEU:HD23	1:B:46:LEU:O	0.43	2.13	15	1
1:A:69:THR:HG21	1:A:101:LEU:CD2	0.43	2.42	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:CD2	1:A:67:MET:HG2	0.43	2.43	4	1
1:B:14:SER:O	1:B:18:TYR:N	0.43	2.49	13	3
1:A:8:LYS:HA	1:A:20:TYR:CA	0.43	2.43	5	1
1:A:98:ILE:HG22	1:A:102:ILE:HD11	0.43	1.89	16	2
1:B:19:PRO:CG	1:B:42:PRO:CD	0.43	2.94	15	2
1:A:7:TYR:C	1:A:81:SER:OG	0.43	2.62	8	1
1:B:30:ASP:C	1:B:35:ARG:HD2	0.43	2.38	8	1
1:A:40:LEU:HD21	1:A:67:MET:HG3	0.43	1.90	9	1
1:B:8:LYS:HG2	1:B:19:PRO:O	0.43	2.12	11	1
1:B:60:ILE:HG21	1:B:87:LEU:HB3	0.43	1.89	11	1
1:B:54:LEU:HD21	1:B:69:THR:HG23	0.43	1.89	12	1
1:B:10:LYS:HB3	1:B:79:ILE:HG22	0.43	1.90	13	1
1:B:35:ARG:CZ	1:B:80:LEU:HD22	0.43	2.43	13	1
1:B:36:LEU:HD12	1:B:72:MET:CG	0.43	2.43	17	1
1:A:105:ILE:C	1:A:105:ILE:HD12	0.43	2.38	19	1
1:A:99:ASP:HA	1:A:103:THR:CG2	0.43	2.43	20	3
1:B:9:ASN:N	1:B:81:SER:HB3	0.43	2.28	4	2
1:B:57:THR:CA	1:B:65:PHE:O	0.43	2.66	17	3
1:A:60:ILE:HD11	1:A:65:PHE:CE1	0.43	2.48	6	1
1:A:4:PHE:CE2	1:A:91:ARG:HB2	0.43	2.48	7	3
1:A:38:ILE:CD1	1:A:67:MET:HB3	0.43	2.43	7	1
1:A:56:PRO:HB2	1:A:93:GLU:HG3	0.43	1.91	10	1
1:A:72:MET:HE1	1:A:98:ILE:HD12	0.43	1.89	15	1
1:A:30:ASP:O	1:A:35:ARG:HD2	0.43	2.14	17	1
1:A:87:LEU:CG	1:A:87:LEU:O	0.43	2.65	1	2
1:B:8:LYS:HG3	1:B:9:ASN:N	0.43	2.28	1	1
1:B:98:ILE:HG22	1:B:99:ASP:N	0.43	2.29	2	4
1:A:84:VAL:HG13	1:A:85:ASN:N	0.43	2.29	3	1
1:B:67:MET:HE1	1:B:93:GLU:CB	0.43	2.44	3	1
1:A:2:SER:HB2	1:A:31:ASN:CB	0.43	2.44	15	2
1:A:25:GLN:CG	1:A:36:LEU:CB	0.43	2.97	16	5
1:B:8:LYS:CG	1:B:9:ASN:ND2	0.43	2.81	15	2
1:B:5:THR:HG23	1:B:86:GLU:HG2	0.43	1.90	9	1
1:A:64:ASP:C	1:A:65:PHE:CD2	0.43	2.96	10	3
1:B:2:SER:O	1:B:30:ASP:CG	0.43	2.60	14	1
1:A:76:PRO:HB3	1:A:78:LYS:CE	0.43	2.44	16	1
1:B:8:LYS:O	1:B:81:SER:C	0.43	2.62	16	1
1:B:23:ASP:HA	1:B:37:VAL:HG12	0.43	1.89	16	1
1:B:38:ILE:CG2	1:B:38:ILE:O	0.43	2.66	2	1
1:A:14:SER:O	1:A:18:TYR:N	0.43	2.45	3	3
1:B:25:GLN:CB	1:B:36:LEU:CB	0.43	2.97	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:LYS:HG3	1:B:79:ILE:C	0.43	2.38	5	2
1:A:9:ASN:CA	1:A:81:SER:HA	0.43	2.44	12	1
1:B:23:ASP:CG	1:B:35:ARG:HB3	0.43	2.39	14	1
1:A:6:LEU:CD2	1:A:87:LEU:HB3	0.43	2.43	20	1
1:A:24:VAL:CG2	1:A:98:ILE:CD1	0.43	2.97	12	3
1:A:82:GLU:O	1:A:83:PRO:C	0.43	2.62	5	3
1:B:64:ASP:C	1:B:65:PHE:CG	0.43	2.96	10	7
1:B:36:LEU:C	1:B:36:LEU:CD1	0.43	2.92	7	2
1:B:6:LEU:O	1:B:6:LEU:CD2	0.43	2.67	15	2
1:B:10:LYS:CB	1:B:79:ILE:O	0.43	2.66	7	2
1:B:20:TYR:CG	1:B:40:LEU:CD1	0.43	3.01	6	1
1:A:5:THR:O	1:A:7:TYR:CE1	0.43	2.72	10	4
1:B:40:LEU:C	1:B:41:THR:HG22	0.43	2.39	12	3
1:B:69:THR:HG22	1:B:101:LEU:HG	0.43	1.90	13	1
1:B:58:ILE:HG13	1:B:90:PHE:CE2	0.43	2.48	3	1
1:A:7:TYR:CZ	1:A:23:ASP:HB2	0.43	2.49	13	5
1:B:10:LYS:HG2	1:B:79:ILE:HG12	0.43	1.89	7	1
1:B:72:MET:HE2	1:B:101:LEU:HD21	0.43	1.91	7	1
1:A:102:ILE:CG2	1:B:102:ILE:HG21	0.43	2.43	8	1
1:B:98:ILE:HG13	1:B:102:ILE:CD1	0.43	2.44	9	1
1:A:3:GLN:O	1:A:4:PHE:CD1	0.43	2.72	11	1
1:A:98:ILE:HG23	1:A:102:ILE:HD11	0.43	1.91	16	1
1:A:54:LEU:CD2	1:A:69:THR:HG22	0.43	2.44	16	2
1:A:90:PHE:CE2	1:A:93:GLU:CD	0.43	2.96	2	4
1:B:10:LYS:CB	1:B:79:ILE:HG22	0.43	2.44	14	5
1:B:59:HIS:CD2	1:B:59:HIS:N	0.43	2.86	3	2
1:B:90:PHE:CE2	1:B:93:GLU:CD	0.43	2.97	11	4
1:A:105:ILE:C	1:A:105:ILE:CD1	0.43	2.92	16	3
1:B:56:PRO:HG2	1:B:67:MET:HE2	0.43	1.91	4	1
1:A:2:SER:CB	1:A:31:ASN:CB	0.43	2.97	6	2
1:B:94:ILE:N	1:B:94:ILE:CD1	0.43	2.82	14	6
1:A:58:ILE:O	1:A:64:ASP:CA	0.43	2.63	10	2
1:B:8:LYS:C	1:B:8:LYS:CD	0.43	2.92	11	1
1:B:25:GLN:CB	1:B:36:LEU:HB3	0.43	2.43	11	2
1:A:31:ASN:O	1:A:31:ASN:OD1	0.43	2.36	12	1
1:B:9:ASN:CB	1:B:14:SER:HB2	0.43	2.44	15	3
1:B:2:SER:HB2	1:B:31:ASN:N	0.43	2.28	5	1
1:B:21:PHE:CD2	1:B:81:SER:HB3	0.43	2.49	5	1
1:A:35:ARG:HG2	1:A:37:VAL:HG13	0.43	1.89	6	1
1:A:2:SER:OG	1:A:31:ASN:ND2	0.43	2.52	7	1
1:B:57:THR:HG23	1:B:65:PHE:O	0.43	2.14	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLN:HA	1:B:74:SER:OG	0.43	2.14	9	1
1:B:24:VAL:O	1:B:25:GLN:CG	0.43	2.67	12	1
1:A:87:LEU:HG	1:A:87:LEU:O	0.43	2.14	13	1
1:A:101:LEU:HD11	1:B:25:GLN:OE1	0.43	2.12	13	3
1:B:41:THR:HG23	1:B:66:ILE:HD12	0.43	1.86	15	1
1:A:36:LEU:CD2	1:B:72:MET:HE2	0.43	2.43	16	1
1:A:22:VAL:CG1	1:A:94:ILE:HG13	0.43	2.43	18	1
1:B:2:SER:HB3	1:B:31:ASN:N	0.43	2.28	18	1
1:A:54:LEU:O	1:A:56:PRO:CD	0.43	2.67	20	1
1:B:10:LYS:CG	1:B:79:ILE:CA	0.43	2.97	20	1
1:B:9:ASN:HA	1:B:81:SER:HA	0.42	1.90	1	1
1:B:19:PRO:HB2	1:B:20:TYR:CZ	0.42	2.49	1	1
1:A:46:LEU:HD23	1:A:46:LEU:O	0.42	2.14	12	2
1:B:8:LYS:C	1:B:81:SER:CB	0.42	2.91	4	3
1:B:21:PHE:CD2	1:B:81:SER:CB	0.42	3.02	5	1
1:A:56:PRO:HD2	1:A:67:MET:HB3	0.42	1.91	6	1
1:A:35:ARG:O	1:A:74:SER:HA	0.42	2.14	7	2
1:A:40:LEU:CD2	1:A:67:MET:CG	0.42	2.97	7	1
1:B:19:PRO:HG2	1:B:20:TYR:CE1	0.42	2.49	11	3
1:A:62:GLU:HB2	1:A:65:PHE:CZ	0.42	2.49	20	2
1:A:40:LEU:CD1	1:A:67:MET:HE3	0.42	2.43	15	1
1:A:8:LYS:CB	1:A:84:VAL:HB	0.42	2.44	18	1
1:A:101:LEU:O	1:A:101:LEU:HD12	0.42	2.13	18	1
1:A:26:SER:HB2	1:A:35:ARG:NE	0.42	2.29	2	1
1:A:20:TYR:HB2	1:A:40:LEU:HD12	0.42	1.91	4	1
1:A:38:ILE:HD12	1:A:72:MET:HG3	0.42	1.90	4	1
1:A:8:LYS:C	1:A:8:LYS:CD	0.42	2.91	5	1
1:B:5:THR:O	1:B:22:VAL:HG13	0.42	2.13	6	1
1:B:21:PHE:HB3	1:B:37:VAL:HB	0.42	1.91	6	1
1:B:2:SER:HB2	1:B:31:ASN:CG	0.42	2.40	18	3
1:A:10:LYS:HA	1:A:82:GLU:CB	0.42	2.44	11	1
1:A:2:SER:OG	1:A:35:ARG:CD	0.42	2.67	12	1
1:A:6:LEU:HD13	1:A:87:LEU:CG	0.42	2.44	17	1
1:A:35:ARG:NH2	1:A:77:VAL:HG23	0.42	2.28	17	1
1:A:57:THR:HG23	1:A:65:PHE:O	0.42	2.14	19	1
1:A:99:ASP:CA	1:A:103:THR:HG23	0.42	2.44	19	1
1:B:87:LEU:O	1:B:87:LEU:HG	0.42	2.13	19	1
1:B:2:SER:HB3	1:B:35:ARG:CD	0.42	2.45	1	1
1:A:38:ILE:CG2	1:A:69:THR:CB	0.42	2.96	2	1
1:A:22:VAL:CG1	1:A:94:ILE:HG21	0.42	2.43	3	1
1:B:10:LYS:CG	1:B:79:ILE:HG13	0.42	2.45	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:PHE:HZ	1:A:95:ILE:HD11	0.42	1.73	12	2
1:A:76:PRO:HB2	1:A:78:LYS:HG2	0.42	1.89	6	1
1:A:72:MET:HE2	1:A:102:ILE:CD1	0.42	2.43	8	1
1:A:30:ASP:HA	1:A:35:ARG:NH2	0.42	2.29	11	1
1:A:67:MET:CE	1:A:94:ILE:CD1	0.42	2.97	12	1
1:B:43:ILE:HG23	1:B:66:ILE:HG23	0.42	1.91	15	1
1:A:102:ILE:HG13	1:A:103:THR:N	0.42	2.28	17	1
1:B:10:LYS:CB	1:B:79:ILE:CG2	0.42	2.98	18	1
1:B:8:LYS:O	1:B:19:PRO:O	0.42	2.37	1	1
1:B:38:ILE:CG1	1:B:67:MET:HB3	0.42	2.45	2	1
1:A:30:ASP:HA	1:A:35:ARG:CG	0.42	2.43	5	2
1:A:100:PHE:HA	1:A:104:GLY:HA2	0.42	1.89	4	1
1:A:51:PRO:O	1:A:53:HIS:N	0.42	2.52	5	1
1:B:84:VAL:HG13	1:B:85:ASN:N	0.42	2.29	12	2
1:B:32:LEU:HD23	1:B:33:ASN:ND2	0.42	2.29	9	1
1:A:101:LEU:HD23	1:A:102:ILE:HG23	0.42	1.90	10	1
1:B:24:VAL:HG13	1:B:98:ILE:CD1	0.42	2.45	11	1
1:B:25:GLN:HG3	1:B:36:LEU:HB3	0.42	1.90	12	1
1:B:69:THR:HG22	1:B:101:LEU:CG	0.42	2.44	13	1
1:B:10:LYS:HD2	1:B:79:ILE:HG13	0.42	1.91	17	1
1:A:35:ARG:CZ	1:A:80:LEU:CD1	0.42	2.97	1	1
1:B:7:TYR:CE1	1:B:23:ASP:OD1	0.42	2.72	17	2
1:B:35:ARG:CG	1:B:36:LEU:N	0.42	2.82	2	1
1:A:8:LYS:HB3	1:A:84:VAL:HG13	0.42	1.91	6	1
1:A:10:LYS:CA	1:A:82:GLU:HB2	0.42	2.45	8	1
1:A:19:PRO:HD2	1:A:40:LEU:O	0.42	2.15	8	3
1:B:75:VAL:HG22	1:B:79:ILE:CD1	0.42	2.44	8	1
1:B:97:ALA:C	1:B:101:LEU:HD23	0.42	2.39	11	2
1:B:31:ASN:CB	1:B:35:ARG:NH2	0.42	2.83	13	1
1:A:17:THR:HG22	1:A:18:TYR:CD1	0.42	2.49	14	1
1:A:25:GLN:O	1:A:27:ASP:N	0.42	2.53	16	1
1:B:31:ASN:HB3	1:B:35:ARG:NH1	0.42	2.30	19	1
1:A:8:LYS:O	1:A:81:SER:HA	0.42	2.15	1	1
1:B:36:LEU:HD13	1:B:74:SER:OG	0.42	2.14	1	1
1:A:58:ILE:HG23	1:A:90:PHE:CE1	0.42	2.50	3	1
1:B:78:LYS:CD	1:B:78:LYS:H	0.42	2.27	4	2
1:A:76:PRO:O	1:A:77:VAL:C	0.42	2.61	17	5
1:B:2:SER:HB2	1:B:31:ASN:CB	0.42	2.45	6	1
1:B:7:TYR:CD2	1:B:80:LEU:HD11	0.42	2.50	6	1
1:A:10:LYS:CE	1:A:79:ILE:HG13	0.42	2.45	8	1
1:A:2:SER:OG	1:A:35:ARG:HD3	0.42	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:100:PHE:CE1	1:B:105:ILE:HD12	0.42	2.49	9	1
1:A:75:VAL:HG23	1:A:80:LEU:HD22	0.42	1.91	10	1
1:A:26:SER:N	1:A:35:ARG:HH21	0.42	2.12	11	1
1:A:8:LYS:HB2	1:A:84:VAL:HG13	0.42	1.90	15	1
1:A:101:LEU:HD23	1:B:25:GLN:NE2	0.42	2.28	15	1
1:B:58:ILE:HG22	1:B:90:PHE:CE2	0.42	2.49	15	1
1:B:2:SER:HB3	1:B:30:ASP:C	0.42	2.39	18	1
1:B:28:LEU:O	1:B:32:LEU:HD12	0.42	2.13	19	1
1:B:7:TYR:CZ	1:B:23:ASP:OD1	0.42	2.73	15	2
1:B:40:LEU:HA	1:B:67:MET:HA	0.42	1.90	2	1
1:B:68:LEU:HD23	1:B:70:GLN:HG3	0.42	1.91	2	1
1:A:6:LEU:CG	1:A:87:LEU:HG	0.42	2.44	3	1
1:A:9:ASN:OD1	1:A:9:ASN:O	0.42	2.37	3	1
1:A:8:LYS:C	1:A:81:SER:CB	0.42	2.92	10	2
1:A:2:SER:O	1:A:30:ASP:OD2	0.42	2.38	5	1
1:B:65:PHE:CD1	1:B:65:PHE:N	0.42	2.88	9	2
1:A:8:LYS:HD2	1:A:20:TYR:CD2	0.42	2.49	15	2
1:A:9:ASN:OD1	1:A:21:PHE:CZ	0.42	2.72	15	3
1:B:43:ILE:CD1	1:B:57:THR:OG1	0.42	2.61	10	1
1:A:101:LEU:CD1	1:B:25:GLN:NE2	0.42	2.82	16	2
1:B:38:ILE:HD13	1:B:67:MET:SD	0.42	2.55	15	1
1:B:24:VAL:O	1:B:25:GLN:HB3	0.42	2.15	17	1
1:A:24:VAL:HG23	1:A:25:GLN:N	0.42	2.29	18	1
1:A:38:ILE:HG23	1:A:69:THR:CG2	0.42	2.44	18	1
1:B:96:ALA:HA	1:B:105:ILE:HG21	0.42	1.90	19	1
1:A:77:VAL:O	1:A:80:LEU:HB2	0.42	2.14	1	1
1:B:6:LEU:HG	1:B:87:LEU:HG	0.42	1.91	1	1
1:B:88:SER:O	1:B:91:ARG:CD	0.42	2.68	15	5
1:A:38:ILE:O	1:A:40:LEU:N	0.42	2.53	2	1
1:B:23:ASP:HA	1:B:35:ARG:CD	0.42	2.45	3	1
1:A:3:GLN:N	1:A:7:TYR:OH	0.42	2.53	4	1
1:A:73:THR:HG22	1:B:73:THR:CB	0.42	2.44	5	1
1:B:78:LYS:H	1:B:78:LYS:CD	0.42	2.27	5	1
1:A:87:LEU:O	1:A:87:LEU:CG	0.42	2.66	13	1
1:A:37:VAL:CG2	1:A:73:THR:O	0.42	2.68	15	2
1:A:35:ARG:CZ	1:A:80:LEU:CD2	0.42	2.97	17	1
1:A:38:ILE:HG21	1:A:67:MET:HG2	0.42	1.90	17	1
1:A:58:ILE:HG12	1:A:90:PHE:CG	0.42	2.49	18	1
1:B:9:ASN:HB2	1:B:14:SER:CB	0.42	2.45	8	1
1:A:80:LEU:O	1:A:80:LEU:HD12	0.42	2.14	9	1
1:A:2:SER:OG	1:A:31:ASN:HB3	0.42	2.15	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD23	1:A:87:LEU:HD21	0.42	1.92	10	1
1:A:36:LEU:CD2	1:B:72:MET:CE	0.42	2.97	14	1
1:A:58:ILE:HD12	1:A:87:LEU:HD11	0.42	1.92	14	1
1:A:94:ILE:CD1	1:A:94:ILE:N	0.42	2.83	17	1
1:A:10:LYS:HG2	1:A:79:ILE:CD1	0.42	2.45	18	1
1:A:46:LEU:CD2	1:A:68:LEU:HD13	0.42	2.45	18	1
1:B:30:ASP:C	1:B:35:ARG:HD3	0.42	2.40	19	1
1:B:19:PRO:HB2	1:B:20:TYR:CD1	0.42	2.49	4	3
1:A:69:THR:OG1	1:A:101:LEU:CB	0.42	2.68	3	1
1:B:31:ASN:O	1:B:32:LEU:C	0.42	2.62	4	3
1:B:2:SER:HB2	1:B:30:ASP:C	0.42	2.40	7	2
1:B:6:LEU:CB	1:B:87:LEU:HD22	0.42	2.45	9	2
1:A:57:THR:CG2	1:A:59:HIS:CE1	0.42	3.03	8	1
1:B:56:PRO:HD2	1:B:67:MET:CB	0.42	2.44	8	3
1:B:76:PRO:O	1:B:79:ILE:CD1	0.42	2.68	8	1
1:A:29:LEU:HD22	1:B:70:GLN:NE2	0.42	2.29	9	1
1:A:25:GLN:HG3	1:B:102:ILE:HG22	0.42	1.91	10	1
1:A:63:GLY:O	1:A:65:PHE:CZ	0.42	2.73	15	1
1:A:26:SER:O	1:A:30:ASP:HB3	0.42	2.13	17	2
1:A:34:THR:HA	1:A:35:ARG:NH2	0.42	2.30	16	1
1:B:42:PRO:CA	1:B:65:PHE:CD2	0.42	3.03	19	1
1:A:31:ASN:CB	1:A:35:ARG:NE	0.42	2.83	20	1
1:B:4:PHE:CZ	1:B:91:ARG:HB2	0.41	2.50	1	2
1:B:69:THR:OG1	1:B:101:LEU:CB	0.41	2.68	2	1
1:B:75:VAL:O	1:B:75:VAL:CG2	0.41	2.68	5	1
1:A:44:GLU:HG3	1:A:48:LYS:CG	0.41	2.45	6	1
1:A:3:GLN:HB2	1:A:35:ARG:NH1	0.41	2.29	7	1
1:B:38:ILE:CD1	1:B:97:ALA:CB	0.41	2.98	7	3
1:A:35:ARG:NH1	1:A:80:LEU:CD2	0.41	2.83	8	1
1:A:72:MET:CE	1:B:36:LEU:CD2	0.41	2.98	9	1
1:B:23:ASP:O	1:B:35:ARG:NH1	0.41	2.53	11	1
1:B:37:VAL:O	1:B:72:MET:CG	0.41	2.67	14	1
1:A:8:LYS:HD3	1:A:20:TYR:CD2	0.41	2.50	15	1
1:A:58:ILE:HD11	1:A:65:PHE:CB	0.41	2.41	15	1
1:B:20:TYR:CZ	1:B:65:PHE:HD2	0.41	2.32	15	1
1:B:24:VAL:O	1:B:24:VAL:CG2	0.41	2.68	15	1
1:A:87:LEU:O	1:A:87:LEU:HG	0.41	2.15	1	1
1:B:7:TYR:O	1:B:21:PHE:N	0.41	2.46	1	1
1:A:7:TYR:CG	1:A:23:ASP:OD1	0.41	2.73	5	1
1:B:6:LEU:CA	1:B:87:LEU:HD22	0.41	2.45	19	2
1:B:35:ARG:NH1	1:B:80:LEU:HD22	0.41	2.29	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ILE:HD12	1:B:67:MET:CE	0.41	2.45	5	1
1:A:8:LYS:HE2	1:A:84:VAL:HG21	0.41	1.92	9	1
1:B:25:GLN:CG	1:B:36:LEU:CB	0.41	2.98	13	2
1:B:2:SER:HB2	1:B:30:ASP:CG	0.41	2.40	11	1
1:B:67:MET:SD	1:B:94:ILE:HD12	0.41	2.54	11	1
1:A:58:ILE:N	1:A:58:ILE:CD1	0.41	2.83	12	1
1:B:7:TYR:CE2	1:B:23:ASP:OD2	0.41	2.73	20	4
1:B:54:LEU:HD21	1:B:69:THR:HG22	0.41	1.91	12	1
1:A:4:PHE:CZ	1:A:95:ILE:CD1	0.41	2.99	14	1
1:B:57:THR:C	1:B:58:ILE:HG12	0.41	2.41	14	1
1:A:6:LEU:O	1:A:6:LEU:CD1	0.41	2.68	15	1
1:B:2:SER:O	1:B:3:GLN:CG	0.41	2.68	20	1
1:A:78:LYS:CD	1:A:78:LYS:H	0.41	2.28	10	3
1:A:94:ILE:N	1:A:94:ILE:CD1	0.41	2.84	9	2
1:B:41:THR:CG2	1:B:68:LEU:HD12	0.41	2.45	2	1
1:A:45:LEU:C	1:A:45:LEU:CD1	0.41	2.91	4	1
1:B:54:LEU:CD2	1:B:101:LEU:HD13	0.41	2.45	4	1
1:B:73:THR:OG1	1:B:74:SER:N	0.41	2.53	4	1
1:B:69:THR:CG2	1:B:101:LEU:HD12	0.41	2.40	6	1
1:B:14:SER:C	1:B:18:TYR:O	0.41	2.63	15	2
1:B:7:TYR:CD2	1:B:80:LEU:HG	0.41	2.51	15	1
1:A:26:SER:O	1:A:27:ASP:C	0.41	2.63	16	1
1:A:74:SER:N	1:B:71:GLN:O	0.41	2.53	17	1
1:A:20:TYR:O	1:A:39:PRO:HA	0.41	2.14	19	1
1:B:7:TYR:CD1	1:B:23:ASP:OD1	0.41	2.74	2	2
1:B:10:LYS:HG3	1:B:79:ILE:HA	0.41	1.92	2	1
1:A:4:PHE:CE2	1:A:91:ARG:NH1	0.41	2.88	3	1
1:A:8:LYS:HB2	1:A:84:VAL:CB	0.41	2.46	3	1
1:B:10:LYS:HG2	1:B:79:ILE:HG13	0.41	1.91	5	1
1:B:6:LEU:CG	1:B:87:LEU:HD13	0.41	2.43	7	2
1:B:38:ILE:HG23	1:B:69:THR:CA	0.41	2.45	8	2
1:B:40:LEU:CD2	1:B:67:MET:HE2	0.41	2.18	8	1
1:A:35:ARG:NH1	1:A:80:LEU:CD1	0.41	2.83	12	1
1:B:43:ILE:CG1	1:B:48:LYS:CD	0.41	2.98	14	1
1:A:26:SER:CB	1:A:35:ARG:CZ	0.41	2.99	2	1
1:A:34:THR:HB	1:A:76:PRO:HA	0.41	1.93	2	1
1:A:58:ILE:HG13	1:A:90:PHE:CE2	0.41	2.51	2	2
1:A:44:GLU:HA	1:A:48:LYS:HD3	0.41	1.93	5	1
1:B:25:GLN:HG3	1:B:36:LEU:HD23	0.41	1.91	12	1
1:B:43:ILE:HG22	1:B:65:PHE:CA	0.41	2.45	20	4
1:B:54:LEU:CD2	1:B:69:THR:HG22	0.41	2.46	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:42:PRO:CG	1:B:45:LEU:HG	0.41	2.45	13	1
1:A:31:ASN:HA	1:A:35:ARG:CD	0.41	2.45	17	1
1:A:5:THR:CG2	1:A:85:ASN:O	0.41	2.69	20	1
1:B:10:LYS:CG	1:B:79:ILE:CB	0.41	2.98	20	1
1:B:20:TYR:CD1	1:B:40:LEU:HB2	0.41	2.50	20	1
1:A:26:SER:HB3	1:A:29:LEU:N	0.41	2.31	16	3
1:A:90:PHE:CE2	1:A:93:GLU:CG	0.41	3.03	2	1
1:B:42:PRO:HG3	1:B:45:LEU:CD2	0.41	2.44	2	1
1:A:25:GLN:N	1:A:35:ARG:NE	0.41	2.69	5	1
1:A:63:GLY:O	1:A:65:PHE:CE2	0.41	2.74	10	1
1:A:24:VAL:CG1	1:A:38:ILE:HD13	0.41	2.46	12	1
1:A:35:ARG:HA	1:A:35:ARG:NH1	0.41	2.31	15	1
1:A:98:ILE:HA	1:A:102:ILE:CD1	0.41	2.45	15	1
1:B:20:TYR:N	1:B:20:TYR:HD1	0.41	2.10	15	1
1:B:25:GLN:CG	1:B:26:SER:N	0.41	2.82	15	1
1:B:25:GLN:HE21	1:B:36:LEU:HD22	0.41	1.75	15	1
1:A:31:ASN:HB2	1:A:77:VAL:HG21	0.41	1.92	18	1
1:A:5:THR:HG23	1:A:86:GLU:CA	0.41	2.45	20	1
1:A:7:TYR:HB3	1:A:81:SER:O	0.41	2.16	20	1
1:A:35:ARG:NE	1:A:80:LEU:CD2	0.41	2.84	20	1
1:B:2:SER:C	1:B:30:ASP:CG	0.41	2.89	20	1
1:A:7:TYR:CG	1:A:35:ARG:NH1	0.41	2.89	1	1
1:A:54:LEU:HD22	1:B:29:LEU:HD11	0.41	1.92	1	1
1:A:25:GLN:HB3	1:A:35:ARG:HH11	0.41	1.76	2	1
1:A:35:ARG:CG	1:A:36:LEU:N	0.41	2.84	2	1
1:A:38:ILE:HD13	1:A:67:MET:HB3	0.41	1.92	7	1
1:B:24:VAL:CB	1:B:94:ILE:HG23	0.41	2.44	7	1
1:A:10:LYS:HE2	1:A:11:ASP:HB2	0.41	1.91	8	1
1:B:88:SER:O	1:B:91:ARG:N	0.41	2.46	8	1
1:A:8:LYS:N	1:A:81:SER:HB2	0.41	2.30	10	1
1:B:9:ASN:OD1	1:B:21:PHE:CE1	0.41	2.74	16	1
1:A:9:ASN:OD1	1:A:14:SER:CB	0.41	2.69	18	1
1:B:38:ILE:CD1	1:B:69:THR:OG1	0.41	2.69	18	1
1:A:31:ASN:HB2	1:A:35:ARG:NE	0.41	2.31	20	1
1:B:10:LYS:O	1:B:82:GLU:CG	0.41	2.69	20	1
1:B:63:GLY:O	1:B:65:PHE:CE2	0.41	2.74	1	1
1:A:42:PRO:HG3	1:A:45:LEU:CD2	0.41	2.46	4	1
1:A:21:PHE:HB2	1:A:37:VAL:CB	0.41	2.45	5	1
1:B:8:LYS:CA	1:B:81:SER:HB2	0.41	2.45	6	1
1:A:25:GLN:HG3	1:B:102:ILE:HG23	0.41	1.93	7	1
1:B:54:LEU:HD21	1:B:101:LEU:HD22	0.41	1.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ILE:HA	1:B:72:MET:HE2	0.41	1.93	8	1
1:A:103:THR:CG2	1:B:103:THR:CG2	0.41	2.99	10	1
1:A:102:ILE:CD1	1:A:103:THR:CG2	0.41	2.97	11	1
1:A:8:LYS:HG3	1:A:9:ASN:N	0.41	2.30	12	1
1:B:35:ARG:NH2	1:B:80:LEU:CD2	0.41	2.80	13	2
1:A:14:SER:C	1:A:18:TYR:O	0.41	2.64	18	1
1:A:34:THR:CA	1:A:35:ARG:NH2	0.41	2.83	19	1
1:B:45:LEU:HD23	1:B:45:LEU:N	0.41	2.30	20	1
1:B:2:SER:OG	1:B:31:ASN:CB	0.41	2.68	1	1
1:B:59:HIS:H	1:B:90:PHE:HE2	0.41	1.59	1	1
1:A:24:VAL:HB	1:A:94:ILE:HG22	0.41	1.92	3	1
1:A:38:ILE:CD1	1:A:97:ALA:CB	0.41	2.99	3	3
1:A:92:ASN:ND2	1:A:93:GLU:N	0.41	2.69	4	4
1:A:46:LEU:O	1:A:46:LEU:HD22	0.41	2.16	4	1
1:B:20:TYR:CD1	1:B:40:LEU:HB3	0.41	2.51	4	1
1:A:8:LYS:HA	1:A:20:TYR:HA	0.41	1.93	5	1
1:A:57:THR:HG23	1:A:58:ILE:N	0.41	2.30	6	1
1:B:25:GLN:HG3	1:B:36:LEU:HB2	0.41	1.93	6	1
1:B:35:ARG:CZ	1:B:80:LEU:CD2	0.41	2.99	6	1
1:A:9:ASN:OD1	1:A:10:LYS:HD2	0.41	2.15	7	1
1:B:69:THR:HG21	1:B:101:LEU:CD2	0.41	2.45	7	1
1:A:54:LEU:HD23	1:A:69:THR:OG1	0.41	2.15	8	1
1:A:75:VAL:CG2	1:A:79:ILE:HG23	0.41	2.46	8	1
1:A:25:GLN:CG	1:A:26:SER:N	0.41	2.84	11	2
1:B:8:LYS:C	1:B:8:LYS:HD2	0.41	2.41	11	1
1:A:8:LYS:HD3	1:A:20:TYR:CE2	0.41	2.51	15	2
1:B:22:VAL:CG2	1:B:67:MET:CE	0.41	2.99	12	1
1:A:101:LEU:CD2	1:B:25:GLN:NE2	0.41	2.84	15	1
1:A:99:ASP:OD2	1:A:105:ILE:HG21	0.41	2.16	16	1
1:B:92:ASN:CG	1:B:93:GLU:N	0.41	2.79	16	1
1:A:31:ASN:CB	1:A:35:ARG:NH1	0.41	2.84	17	1
1:B:3:GLN:HA	1:B:23:ASP:CB	0.41	2.46	17	1
1:B:7:TYR:CE1	1:B:23:ASP:CG	0.41	2.99	17	1
1:B:9:ASN:ND2	1:B:14:SER:CB	0.41	2.84	17	1
1:B:35:ARG:NH1	1:B:80:LEU:CD1	0.41	2.84	17	1
1:A:25:GLN:HE21	1:B:101:LEU:HD11	0.41	1.68	18	1
1:A:2:SER:HB3	1:A:31:ASN:CB	0.41	2.46	19	1
1:A:7:TYR:HB3	1:A:81:SER:OG	0.41	2.16	19	1
1:A:6:LEU:HD12	1:A:84:VAL:CG2	0.41	2.36	20	1
1:B:92:ASN:ND2	1:B:93:GLU:N	0.41	2.69	2	3
1:A:69:THR:HG1	1:A:101:LEU:HD22	0.41	1.72	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:LEU:CD2	1:B:32:LEU:HD13	0.41	2.42	3	1
1:B:75:VAL:HG22	1:B:80:LEU:HA	0.41	1.93	3	1
1:A:87:LEU:H	1:A:87:LEU:CD2	0.41	2.28	20	2
1:B:21:PHE:CA	1:B:39:PRO:HA	0.41	2.46	7	1
1:B:41:THR:C	1:B:66:ILE:HD12	0.41	2.40	7	1
1:A:6:LEU:C	1:A:6:LEU:CD2	0.41	2.94	9	1
1:A:79:ILE:C	1:A:81:SER:H	0.41	2.23	11	1
1:A:31:ASN:ND2	1:A:35:ARG:NH1	0.41	2.69	12	1
1:A:35:ARG:CD	1:A:80:LEU:CD1	0.41	2.99	12	1
1:B:42:PRO:C	1:B:44:GLU:N	0.41	2.78	14	2
1:A:2:SER:CB	1:A:31:ASN:CG	0.41	2.94	18	1
1:A:11:ASP:O	1:A:14:SER:HB2	0.40	2.16	1	2
1:B:15:ALA:HA	1:B:19:PRO:HA	0.40	1.94	9	4
1:B:21:PHE:HB3	1:B:37:VAL:CG2	0.40	2.46	1	1
1:A:9:ASN:N	1:A:81:SER:HB3	0.40	2.30	4	1
1:B:75:VAL:O	1:B:75:VAL:HG23	0.40	2.16	7	1
1:B:42:PRO:CG	1:B:45:LEU:CD1	0.40	3.00	8	1
1:A:20:TYR:CD1	1:A:40:LEU:HB2	0.40	2.51	10	1
1:A:69:THR:CB	1:A:101:LEU:HD22	0.40	2.45	12	1
1:A:38:ILE:CD1	1:A:94:ILE:CG2	0.40	2.99	13	2
1:A:22:VAL:HG22	1:A:40:LEU:HD21	0.40	1.91	16	1
1:A:35:ARG:CD	1:A:80:LEU:HD21	0.40	2.45	16	1
1:A:22:VAL:O	1:A:24:VAL:CG1	0.40	2.65	18	1
1:A:11:ASP:C	1:A:13:SER:N	0.40	2.79	19	1
1:A:58:ILE:HD11	1:A:60:ILE:HG12	0.40	1.91	19	1
1:A:9:ASN:CG	1:A:14:SER:OG	0.40	2.64	1	1
1:A:64:ASP:O	1:A:65:PHE:CG	0.40	2.73	10	2
1:B:28:LEU:N	1:B:28:LEU:CD2	0.40	2.84	20	2
1:A:17:THR:HG22	1:A:18:TYR:CE2	0.40	2.51	2	1
1:A:102:ILE:HG23	1:B:25:GLN:CD	0.40	2.41	2	1
1:B:54:LEU:O	1:B:69:THR:HG22	0.40	2.16	2	1
1:A:90:PHE:CE2	1:A:93:GLU:OE1	0.40	2.74	3	1
1:B:37:VAL:O	1:B:72:MET:HE2	0.40	2.15	8	1
1:A:2:SER:N	1:A:30:ASP:OD2	0.40	2.54	9	1
1:A:94:ILE:N	1:A:94:ILE:HD12	0.40	2.32	9	1
1:A:28:LEU:N	1:A:28:LEU:CD2	0.40	2.85	10	2
1:A:72:MET:CE	1:A:101:LEU:HD22	0.40	2.45	10	1
1:A:102:ILE:CD1	1:B:102:ILE:HD13	0.40	2.46	11	1
1:A:101:LEU:HD11	1:B:25:GLN:HE22	0.40	1.74	12	1
1:B:56:PRO:HD2	1:B:67:MET:HB3	0.40	1.93	14	1
1:B:43:ILE:CG2	1:B:66:ILE:CG1	0.40	2.98	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:THR:C	1:A:58:ILE:HG12	0.40	2.41	17	1
1:B:3:GLN:HG2	1:B:4:PHE:CD1	0.40	2.51	17	1
1:A:52:SER:O	1:A:53:HIS:CG	0.40	2.75	19	1
1:B:10:LYS:CA	1:B:82:GLU:HB2	0.40	2.47	1	1
1:B:54:LEU:HD12	1:B:54:LEU:N	0.40	2.32	1	1
1:A:24:VAL:CB	1:A:94:ILE:HG22	0.40	2.46	3	1
1:B:67:MET:HE1	1:B:93:GLU:HG2	0.40	1.93	3	1
1:A:3:GLN:CB	1:A:23:ASP:O	0.40	2.69	9	1
1:A:23:ASP:OD2	1:A:35:ARG:HD2	0.40	2.16	9	2
1:A:88:SER:O	1:A:91:ARG:N	0.40	2.47	9	1
1:A:8:LYS:HB2	1:A:20:TYR:CD2	0.40	2.52	10	1
1:A:9:ASN:C	1:A:11:ASP:H	0.40	2.24	10	1
1:A:24:VAL:CA	1:A:35:ARG:NH1	0.40	2.84	10	1
1:A:105:ILE:CD1	1:A:105:ILE:C	0.40	2.94	10	1
1:A:35:ARG:CZ	1:A:80:LEU:HD12	0.40	2.46	12	1
1:A:74:SER:CB	1:B:71:GLN:O	0.40	2.69	13	1
1:B:9:ASN:OD1	1:B:10:LYS:HD2	0.40	2.16	13	1
1:B:9:ASN:OD1	1:B:10:LYS:CE	0.40	2.69	13	1
1:A:46:LEU:C	1:A:47:ASP:CG	0.40	2.90	14	1
1:B:20:TYR:O	1:B:39:PRO:HA	0.40	2.17	15	1
1:A:35:ARG:NH2	1:A:77:VAL:N	0.40	2.70	16	1
1:B:43:ILE:HG22	1:B:65:PHE:HA	0.40	1.93	16	1
1:A:54:LEU:CD2	1:A:70:GLN:N	0.40	2.84	18	1
1:A:96:ALA:O	1:A:100:PHE:HB3	0.40	2.16	20	1
1:B:20:TYR:CD1	1:B:40:LEU:CB	0.40	3.04	20	1
1:B:45:LEU:N	1:B:45:LEU:CD2	0.40	2.84	20	1
1:B:20:TYR:CD2	1:B:84:VAL:HG11	0.40	2.51	3	1
1:A:38:ILE:CB	1:A:67:MET:HE2	0.40	2.40	4	1
1:B:7:TYR:CZ	1:B:23:ASP:HB3	0.40	2.51	4	1
1:B:8:LYS:HA	1:B:19:PRO:O	0.40	2.16	4	1
1:A:8:LYS:O	1:A:81:SER:C	0.40	2.65	6	1
1:A:92:ASN:CG	1:A:93:GLU:N	0.40	2.79	19	2
1:A:2:SER:O	1:A:35:ARG:HD3	0.40	2.16	7	1
1:A:19:PRO:HB2	1:A:20:TYR:CD1	0.40	2.52	8	1
1:B:66:ILE:HD12	1:B:66:ILE:H	0.40	1.76	8	1
1:A:65:PHE:O	1:A:66:ILE:HG23	0.40	2.16	9	1
1:A:22:VAL:HG22	1:A:40:LEU:HD11	0.40	1.93	11	1
1:A:36:LEU:HD13	1:A:74:SER:OG	0.40	2.16	11	1
1:A:35:ARG:NH1	1:A:80:LEU:HD12	0.40	2.32	12	1
1:A:23:ASP:HB3	1:A:35:ARG:CZ	0.40	2.46	13	1
1:A:9:ASN:ND2	1:A:14:SER:CB	0.40	2.85	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ARG:CZ	1:A:80:LEU:HG	0.40	2.46	16	1
1:B:41:THR:HG21	1:B:68:LEU:CD1	0.40	2.46	18	1
1:B:99:ASP:OD2	1:B:105:ILE:HD12	0.40	2.14	19	1
1:B:35:ARG:HD2	1:B:80:LEU:HD11	0.40	1.94	1	1
1:A:69:THR:OG1	1:A:72:MET:CE	0.40	2.68	2	1
1:B:75:VAL:HG13	1:B:80:LEU:HD13	0.40	1.94	2	1
1:B:23:ASP:OD2	1:B:35:ARG:CD	0.40	2.69	4	1
1:B:98:ILE:HG12	1:B:102:ILE:HD12	0.40	1.93	5	1
1:B:35:ARG:CD	1:B:80:LEU:CD2	0.40	3.00	6	1
1:B:84:VAL:HG23	1:B:85:ASN:N	0.40	2.31	6	1
1:B:66:ILE:N	1:B:66:ILE:CD1	0.40	2.85	7	1
1:B:9:ASN:CB	1:B:14:SER:CB	0.40	2.99	8	1
1:B:23:ASP:CG	1:B:35:ARG:HG2	0.40	2.41	8	1
1:B:58:ILE:HG22	1:B:90:PHE:CD2	0.40	2.51	8	1
1:A:24:VAL:N	1:A:35:ARG:HH11	0.40	2.15	10	1
1:B:36:LEU:CD2	1:B:72:MET:CE	0.40	3.00	10	1
1:A:101:LEU:HD12	1:B:25:GLN:CD	0.40	2.41	11	1
1:A:19:PRO:HB2	1:A:20:TYR:CZ	0.40	2.52	14	1
1:A:20:TYR:CD2	1:A:84:VAL:HG11	0.40	2.51	14	1
1:B:54:LEU:HD11	1:B:101:LEU:HA	0.40	1.93	14	1
1:A:2:SER:HB3	1:A:31:ASN:HB3	0.40	1.94	16	1
1:A:10:LYS:CB	1:A:79:ILE:CG2	0.40	3.00	17	1
1:B:6:LEU:HB3	1:B:85:ASN:C	0.40	2.41	18	1
1:A:24:VAL:HG13	1:A:24:VAL:O	0.40	2.16	19	1
1:B:3:GLN:NE2	1:B:4:PHE:CE2	0.40	2.90	19	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/105 (98%)	65±15 (63±15%)	22±6 (21±6%)	11±3 (11±3%)	1	8
1	B	103/105 (98%)	67±4 (65±4%)	24±3 (23±3%)	11±3 (10±3%)	1	9
All	All	3993/4200 (95%)	2637 (66%)	912 (23%)	444 (11%)	1	8

All 51 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	10	LYS	19
1	A	19	PRO	19
1	A	25	GLN	19
1	B	10	LYS	19
1	B	19	PRO	19
1	B	25	GLN	19
1	A	81	SER	18
1	B	81	SER	18
1	A	39	PRO	17
1	B	39	PRO	16
1	B	9	ASN	16
1	A	83	PRO	15
1	A	9	ASN	14
1	B	83	PRO	14
1	B	80	LEU	14
1	A	72	MET	13
1	A	3	GLN	12
1	A	80	LEU	12
1	B	47	ASP	12
1	B	72	MET	11
1	A	47	ASP	10
1	B	77	VAL	10
1	B	3	GLN	9
1	B	24	VAL	8
1	A	24	VAL	7
1	B	12	LYS	7
1	A	49	LYS	7
1	A	77	VAL	7
1	A	53	HIS	6
1	B	97	ALA	6
1	A	12	LYS	6
1	A	8	LYS	5
1	A	97	ALA	5
1	A	26	SER	4
1	B	26	SER	4
1	A	2	SER	3
1	B	53	HIS	3
1	A	54	LEU	3
1	A	76	PRO	2
1	B	8	LYS	2
1	B	33	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	B	49	LYS	2
1	A	4	PHE	2
1	A	55	CYS	1
1	B	32	LEU	1
1	B	54	LEU	1
1	A	52	SER	1
1	A	66	ILE	1
1	B	99	ASP	1
1	B	2	SER	1
1	B	51	PRO	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	98/99 (99%)	60±4 (61±4%)	37±4 (38±4%)	0 7
1	B	99/99 (100%)	61±4 (61±4%)	38±4 (39±4%)	0 6
All	All	3915/3960 (99%)	2402 (61%)	1513 (39%)	0 6

All 154 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	41	THR	20
1	A	48	LYS	20
1	A	66	ILE	20
1	A	78	LYS	20
1	A	79	ILE	20
1	A	87	LEU	20
1	A	93	GLU	20
1	B	5	THR	20
1	B	10	LYS	20
1	B	20	TYR	20
1	B	21	PHE	20
1	B	41	THR	20
1	B	48	LYS	20
1	B	66	ILE	20

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Mol	Chain	Res	Type	Models (Total)
1	B	78	LYS	20
1	B	87	LEU	20
1	B	101	LEU	20
1	A	10	LYS	19
1	A	12	LYS	19
1	A	20	TYR	19
1	A	21	PHE	19
1	A	35	ARG	19
1	A	58	ILE	19
1	A	101	LEU	19
1	B	58	ILE	19
1	B	81	SER	19
1	B	93	GLU	19
1	A	5	THR	18
1	B	14	SER	18
1	B	32	LEU	18
1	B	79	ILE	18
1	A	32	LEU	17
1	A	91	ARG	17
1	B	57	THR	17
1	A	69	THR	17
1	A	81	SER	17
1	A	92	ASN	17
1	A	14	SER	16
1	B	80	LEU	16
1	B	8	LYS	16
1	B	92	ASN	16
1	B	35	ARG	15
1	B	82	GLU	15
1	A	82	GLU	14
1	B	12	LYS	14
1	B	68	LEU	14
1	B	69	THR	14
1	A	57	THR	14
1	A	80	LEU	13
1	B	91	ARG	13
1	A	105	ILE	13
1	B	73	THR	13
1	B	105	ILE	13
1	A	47	ASP	12
1	A	68	LEU	12
1	B	7	TYR	12

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Mol	Chain	Res	Type	Models (Total)
1	A	75	VAL	12
1	A	98	ILE	11
1	A	103	THR	11
1	B	11	ASP	11
1	B	47	ASP	11
1	A	7	TYR	11
1	A	9	ASN	11
1	B	9	ASN	11
1	A	8	LYS	10
1	A	11	ASP	10
1	A	34	THR	10
1	B	72	MET	10
1	A	49	LYS	10
1	A	54	LEU	10
1	A	73	THR	10
1	A	74	SER	10
1	B	38	ILE	10
1	A	2	SER	10
1	B	49	LYS	10
1	B	25	GLN	9
1	B	75	VAL	9
1	B	103	THR	9
1	A	6	LEU	9
1	B	88	SER	9
1	A	85	ASN	9
1	B	2	SER	9
1	A	88	SER	9
1	B	34	THR	8
1	B	43	ILE	8
1	B	3	GLN	8
1	A	38	ILE	7
1	A	72	MET	7
1	B	40	LEU	7
1	B	46	LEU	7
1	B	54	LEU	7
1	B	102	ILE	7
1	A	52	SER	7
1	B	62	GLU	7
1	B	71	GLN	7
1	A	67	MET	6
1	B	98	ILE	6
1	A	46	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	B	24	VAL	6
1	B	67	MET	6
1	A	3	GLN	5
1	B	52	SER	5
1	B	85	ASN	5
1	B	94	ILE	5
1	A	90	PHE	5
1	A	24	VAL	5
1	A	102	ILE	5
1	B	1	MET	5
1	B	90	PHE	5
1	B	44	GLU	5
1	B	74	SER	5
1	A	64	ASP	5
1	A	60	ILE	5
1	B	28	LEU	5
1	A	25	GLN	4
1	A	83	PRO	4
1	B	86	GLU	4
1	B	13	SER	4
1	A	28	LEU	3
1	B	6	LEU	3
1	A	30	ASP	3
1	A	40	LEU	3
1	B	45	LEU	3
1	B	53	HIS	3
1	A	94	ILE	3
1	A	86	GLU	3
1	A	26	SER	3
1	A	31	ASN	3
1	A	16	LYS	2
1	B	26	SER	2
1	A	45	LEU	2
1	A	70	GLN	2
1	A	84	VAL	2
1	B	30	ASP	2
1	B	16	LYS	2
1	A	62	GLU	2
1	A	44	GLU	2
1	B	99	ASP	2
1	B	23	ASP	2
1	B	60	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	99	ASP	2
1	B	36	LEU	2
1	A	27	ASP	1
1	A	71	GLN	1
1	B	77	VAL	1
1	A	53	HIS	1
1	A	61	ASP	1
1	B	31	ASN	1
1	B	61	ASP	1
1	B	70	GLN	1
1	B	84	VAL	1
1	A	36	LEU	1
1	B	29	LEU	1
1	A	55	CYS	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 41% for the well-defined parts and 40% 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	1186
Number of shifts mapped to atoms	1186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	104	0.13 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	100	0.27 ± 0.19	None needed (< 0.5 ppm)
$^{13}C'$	103	0.25 ± 0.18	None needed (< 0.5 ppm)
^{15}N	94	0.50 ± 0.52	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 41%, i.e. 1186 atoms were assigned a chemical shift out of a possible 2919. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	495/1021 (48%)	194/408 (48%)	207/418 (50%)	94/195 (48%)
Sidechain	655/1712 (38%)	426/1123 (38%)	225/545 (41%)	4/44 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	36/186 (19%)	18/90 (20%)	18/88 (20%)	0/8 (0%)
Overall	1186/2919 (41%)	638/1621 (39%)	450/1051 (43%)	98/247 (40%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 1186 atoms were assigned a chemical shift out of a possible 2934. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	495/1026 (48%)	194/410 (47%)	207/420 (49%)	94/196 (48%)
Sidechain	655/1722 (38%)	426/1130 (38%)	225/548 (41%)	4/44 (9%)
Aromatic	36/186 (19%)	18/90 (20%)	18/88 (20%)	0/8 (0%)
Overall	1186/2934 (40%)	638/1630 (39%)	450/1056 (43%)	98/248 (40%)

7.1.4 Statistically unusual chemical shifts (i)

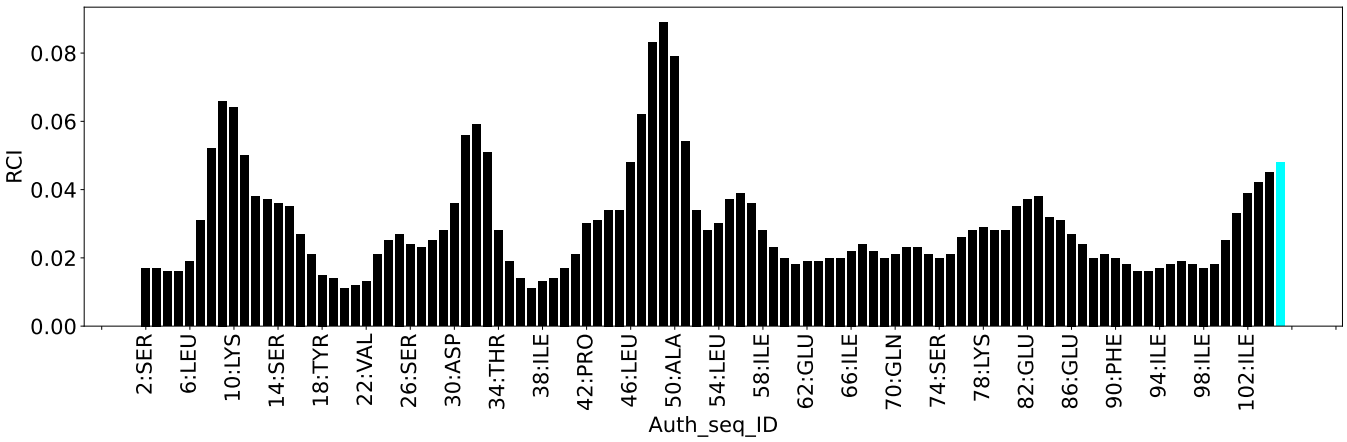
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	41	THR	CG2	15.70	16.06 – 27.03	-5.3

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:


RCI
0.00
0.02
0.04
0.06
0.08
2:SER
6:LEU
10:LYS
14:SER
18:TYR
22:VAL
26:SER
30:ASP
34:THR
38:ILE
42:PRO
46:LEU
50:ALA
54:LEU
58:ILE
62:GLU
66:ILE
70:GLN
74:SER
78:LYS
82:GLU
86:GLU
90:PHE
94:ILE
98:ILE
102:ILE
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3298
Intra-residue (|i-j|=0)	1604
Sequential (|i-j|=1)	494
Medium range (|i-j|>1 and |i-j|<5)	346
Long range (|i-j|≥5)	840
Inter-chain	14
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	278
Number of unmapped restraints	0
Number of restraints per residue	17.0
Number of long range restraints per residue[1]	4.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	86.6	0.2
0.2-0.5 (Medium)	156.6	0.5
>0.5 (Large)	43.1	1.62

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)	28.2	4.78
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

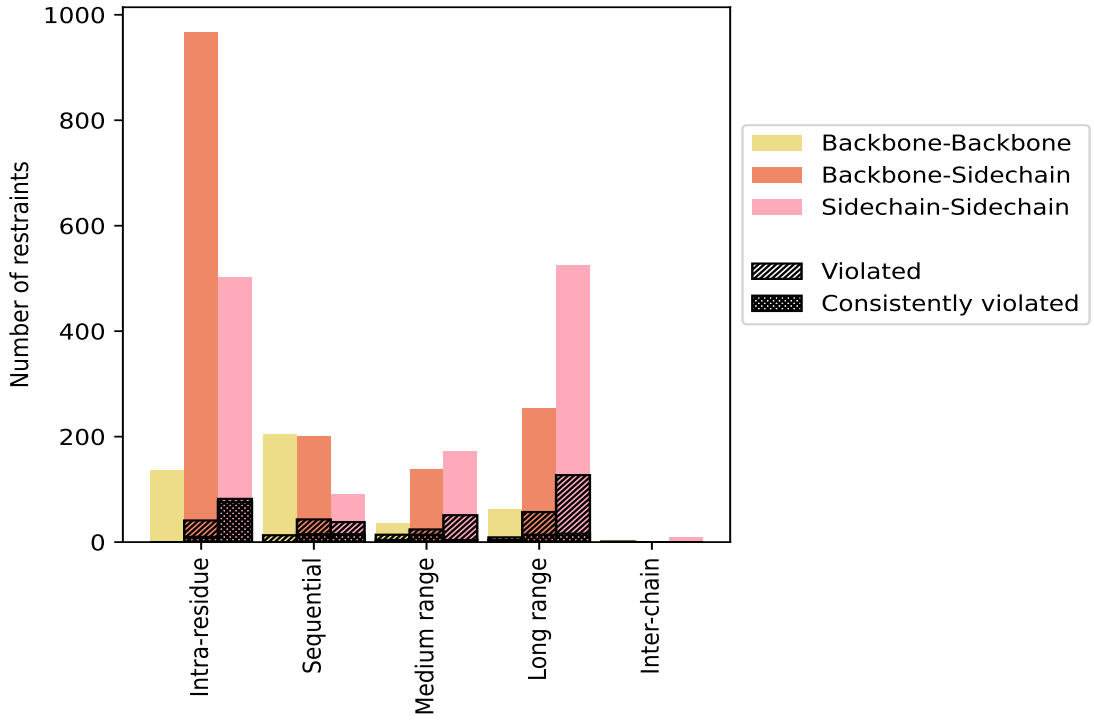
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1604	48.6	123	7.7	3.7	86	5.4	2.6
Backbone-Backbone	136	4.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	966	29.3	41	4.2	1.2	10	1.0	0.3
Sidechain-Sidechain	502	15.2	82	16.3	2.5	76	15.1	2.3
Sequential (|i-j|=1)	494	15.0	94	19.0	2.9	30	6.1	0.9
Backbone-Backbone	204	6.2	13	6.4	0.4	0	0.0	0.0
Backbone-Sidechain	200	6.1	43	21.5	1.3	15	7.5	0.5
Sidechain-Sidechain	90	2.7	38	42.2	1.2	15	16.7	0.5
Medium range (|i-j|>1 & |i-j|<5)	346	10.5	89	25.7	2.7	22	6.4	0.7
Backbone-Backbone	36	1.1	14	38.9	0.4	4	11.1	0.1
Backbone-Sidechain	138	4.2	24	17.4	0.7	14	10.1	0.4
Sidechain-Sidechain	172	5.2	51	29.7	1.5	4	2.3	0.1
Long range (|i-j|≥5)	840	25.5	193	23.0	5.9	34	4.0	1.0
Backbone-Backbone	62	1.9	9	14.5	0.3	4	6.5	0.1
Backbone-Sidechain	254	7.7	57	22.4	1.7	14	5.5	0.4
Sidechain-Sidechain	524	15.9	127	24.2	3.9	16	3.1	0.5
Inter-chain	14	0.4	1	7.1	0.0	0	0.0	0.0
Backbone-Backbone	4	0.1	1	25.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	8	0.2	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	3298	100.0	500	15.2	15.2	172	5.2	5.2
Backbone-Backbone	442	13.4	37	8.4	1.1	8	1.8	0.2
Backbone-Sidechain	1560	47.3	165	10.6	5.0	53	3.4	1.6
Sidechain-Sidechain	1296	39.3	298	23.0	9.0	111	8.6	3.4

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	102	52	55	97	0	306	0.29	1.24	0.19	0.23
2	100	51	46	93	0	290	0.3	1.07	0.2	0.23
3	93	52	49	88	0	282	0.3	1.15	0.2	0.23
4	100	55	49	87	0	291	0.29	1.21	0.19	0.23
5	104	55	46	95	0	300	0.3	1.28	0.2	0.23
6	101	59	50	98	0	308	0.3	1.33	0.21	0.23
7	99	55	48	89	0	291	0.31	1.46	0.2	0.23
8	100	56	47	91	1	295	0.3	1.34	0.2	0.23
9	99	56	47	90	0	292	0.3	1.39	0.21	0.23
10	104	59	47	98	0	308	0.29	1.06	0.18	0.23

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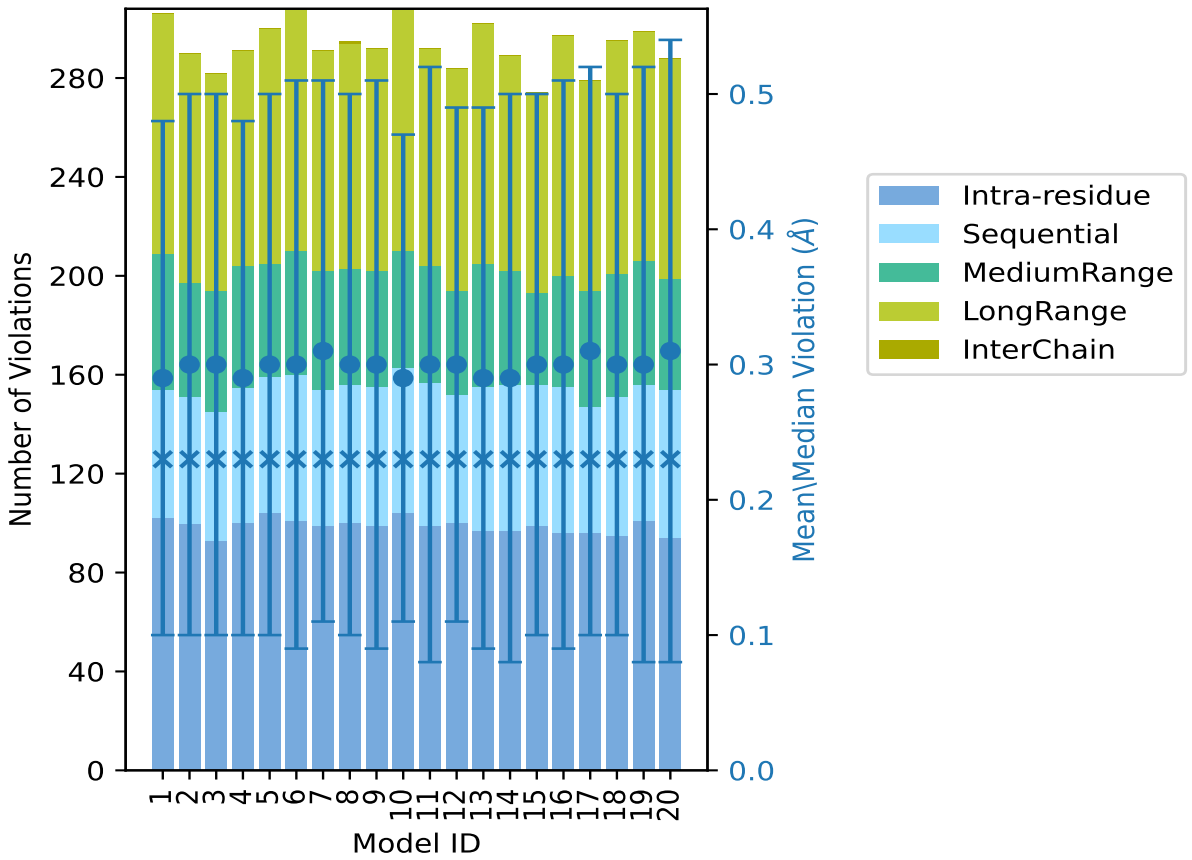
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	99	58	47	88	0	292	0.3	1.47	0.22	0.23
12	100	52	42	90	0	284	0.3	1.27	0.19	0.23
13	97	58	50	97	0	302	0.29	1.35	0.2	0.23
14	97	59	46	87	0	289	0.29	1.35	0.21	0.23
15	99	57	37	81	0	274	0.3	1.49	0.2	0.23
16	96	59	45	97	0	297	0.3	1.39	0.21	0.23
17	96	51	47	85	0	279	0.31	1.23	0.21	0.23
18	95	56	50	94	0	295	0.3	1.13	0.2	0.23
19	101	55	50	93	0	299	0.3	1.57	0.22	0.23
20	94	60	45	89	0	288	0.31	1.62	0.23	0.23

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

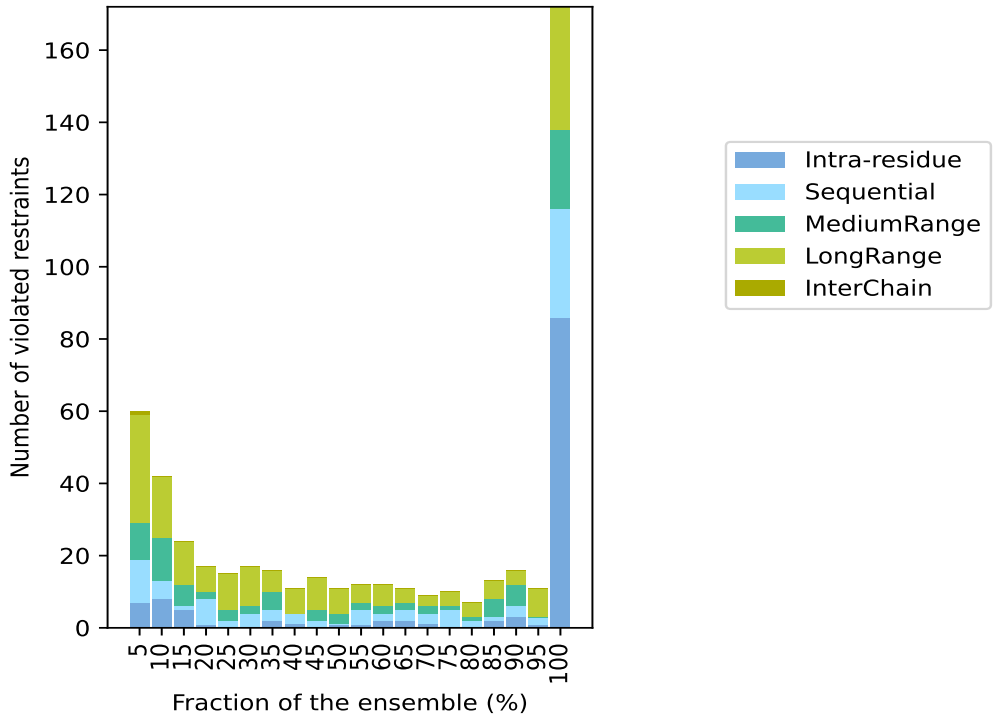
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2798(IR:1481, SQ:400, MR:257, LR:647, IC:13) 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]	%
7	12	10	30	1	60	1	5.0
8	5	12	17	0	42	2	10.0
5	1	6	12	0	24	3	15.0
1	7	2	7	0	17	4	20.0
0	2	3	10	0	15	5	25.0
0	4	2	11	0	17	6	30.0
2	3	5	6	0	16	7	35.0
1	3	0	7	0	11	8	40.0
0	2	3	9	0	14	9	45.0
1	0	3	7	0	11	10	50.0
1	4	2	5	0	12	11	55.0
2	2	2	6	0	12	12	60.0
2	3	2	4	0	11	13	65.0
1	3	2	3	0	9	14	70.0
0	5	1	4	0	10	15	75.0
0	2	1	4	0	7	16	80.0
2	1	5	5	0	13	17	85.0
3	3	6	4	0	16	18	90.0
1	2	0	8	0	11	19	95.0
86	30	22	34	0	172	20	100.0

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

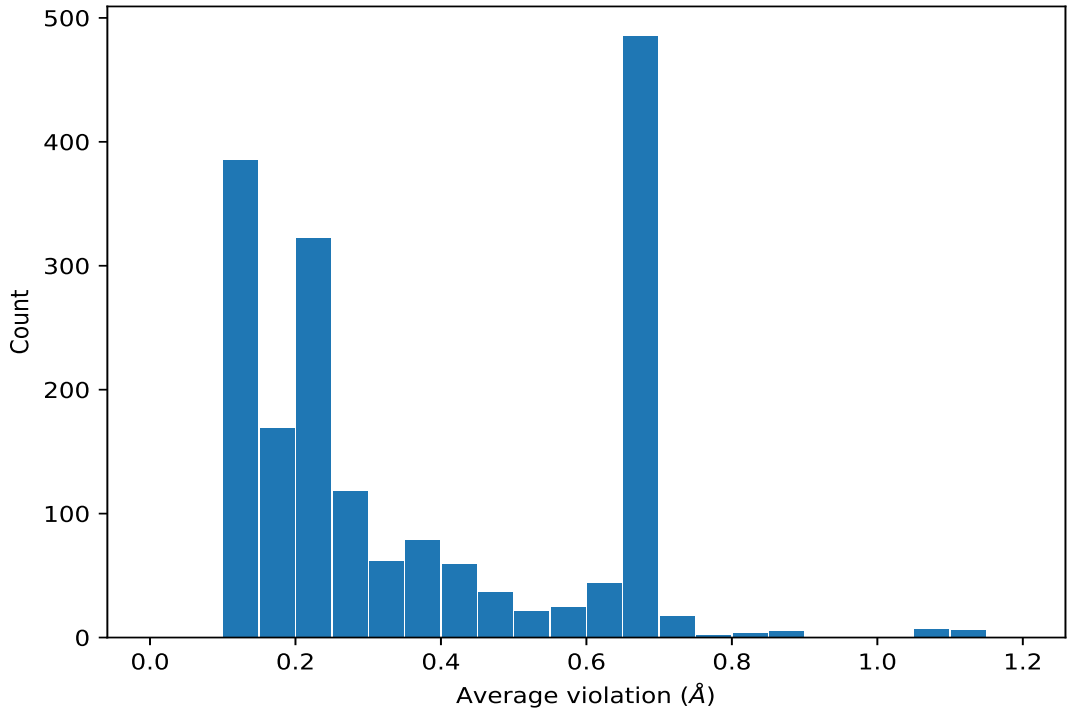
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG12	20	1.11	0.41	1.23
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	20	1.11	0.41	1.23
(1,2031)	1:93:B:GLU:HG3	1:94:B:ILE:HG13	20	1.11	0.41	1.23
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	20	1.08	0.16	1.06
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	20	1.08	0.16	1.06
(1,942)	1:17:A:THR:HG21	1:41:A:THR:HG1	20	1.08	0.16	1.06
(1,2326)	1:17:B:THR:HG21	1:41:B:THR:HG1	20	1.05	0.14	1.04
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	20	1.05	0.14	1.04
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	20	1.05	0.14	1.04
(1,2326)	1:17:B:THR:HG1	1:41:B:THR:HG1	20	1.05	0.14	1.04
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	20	0.87	0.15	0.86
(1,2465)	1:68:B:LEU:HD12	1:66:B:ILE:HG12	20	0.87	0.15	0.86
(1,2465)	1:68:B:LEU:HD13	1:66:B:ILE:HG12	20	0.87	0.15	0.86
(1,2465)	1:68:B:LEU:HD23	1:66:B:ILE:HG12	20	0.87	0.15	0.86
(1,2465)	1:68:B:LEU:HD21	1:66:B:ILE:HG12	20	0.87	0.15	0.86
(1,1081)	1:68:A:LEU:HD13	1:66:A:ILE:HG12	20	0.82	0.17	0.82

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	20	0.82	0.17	0.82
(1,1081)	1:68:A:LEU:HD21	1:66:A:ILE:HG12	20	0.82	0.17	0.82
(1,1081)	1:68:A:LEU:HD12	1:66:A:ILE:HG12	20	0.82	0.17	0.82
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	20	0.65	0.0	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	20	0.65	0.0	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	20	0.65	0.0	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	20	0.65	0.0	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	20	0.65	0.0	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	20	0.65	0.0	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	20	0.65	0.0	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	20	0.65	0.0	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	20	0.65	0.0	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	20	0.65	0.0	0.65

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	20	0.65	0.0	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	20	0.65	0.0	0.65
(1,587)	1:60:A:ILE:HG21	1:90:A:PHE:HZ	20	0.63	0.15	0.57
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	20	0.63	0.15	0.57
(1,587)	1:60:A:ILE:HG13	1:90:A:PHE:HZ	20	0.63	0.15	0.57
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	20	0.61	0.15	0.66
(1,2697)	1:69:B:THR:HG1	1:98:B:ILE:HA	20	0.61	0.15	0.66
(1,2697)	1:69:B:THR:HG21	1:98:B:ILE:HA	20	0.61	0.15	0.66
(1,2697)	1:69:B:THR:HG22	1:98:B:ILE:HA	20	0.61	0.15	0.66
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	20	0.59	0.16	0.58
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	20	0.59	0.16	0.58
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG21	20	0.59	0.16	0.58
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG21	20	0.56	0.14	0.55
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	20	0.56	0.14	0.55
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	20	0.56	0.14	0.55
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG1	20	0.56	0.14	0.55
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	20	0.54	0.06	0.53
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	20	0.54	0.08	0.54
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG23	20	0.54	0.08	0.54
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG13	20	0.54	0.08	0.54
(1,1313)	1:69:A:THR:HG22	1:98:A:ILE:HA	20	0.53	0.14	0.52
(1,1313)	1:69:A:THR:HG1	1:98:A:ILE:HA	20	0.53	0.14	0.52
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	20	0.53	0.14	0.52

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1313)	1:69:A:THR:HG21	1:98:A:ILE:HA	20	0.53	0.14	0.52
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG21	20	0.52	0.18	0.57
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG23	20	0.52	0.18	0.57
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG22	20	0.52	0.18	0.57
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG22	20	0.52	0.18	0.57
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	20	0.52	0.18	0.57
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG21	20	0.52	0.18	0.57
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	20	0.5	0.07	0.5
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG21	20	0.5	0.07	0.5
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG23	20	0.5	0.07	0.5
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG22	20	0.5	0.07	0.5
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	20	0.49	0.07	0.47
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG22	20	0.49	0.07	0.47
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG23	20	0.49	0.07	0.47
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	20	0.49	0.14	0.51
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG22	20	0.49	0.14	0.51
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG23	20	0.49	0.14	0.51
(1,1403)	1:6:B:LEU:HB2	1:5:B:THR:HG21	20	0.49	0.14	0.51
(1,1403)	1:6:B:LEU:HB2	1:5:B:THR:HG23	20	0.49	0.14	0.51
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	20	0.46	0.11	0.45
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	20	0.46	0.11	0.45
(1,1853)	1:11:B:ASP:HB3	1:79:B:ILE:HG21	20	0.46	0.11	0.45
(1,1853)	1:11:B:ASP:HB3	1:79:B:ILE:HG13	20	0.46	0.11	0.45
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	20	0.45	0.11	0.39
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	20	0.45	0.11	0.39
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	20	0.41	0.0	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	20	0.41	0.0	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	20	0.41	0.0	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	20	0.41	0.0	0.41
(1,1190)	1:5:A:THR:HG22	1:83:A:PRO:HG3	20	0.37	0.05	0.37
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	20	0.37	0.05	0.37
(1,1190)	1:5:A:THR:HG23	1:83:A:PRO:HG3	20	0.37	0.05	0.37
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	20	0.37	0.18	0.34
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG21	20	0.37	0.18	0.34
(1,2110)	1:101:B:LEU:HB2	1:102:B:ILE:HG21	20	0.37	0.18	0.34
(1,309)	1:57:A:THR:HG23	1:58:A:ILE:HA	20	0.37	0.03	0.38
(1,309)	1:57:A:THR:HG21	1:58:A:ILE:HA	20	0.37	0.03	0.38
(1,309)	1:57:A:THR:HG22	1:58:A:ILE:HA	20	0.37	0.03	0.38
(1,309)	1:57:A:THR:HG1	1:58:A:ILE:HA	20	0.37	0.03	0.38
(1,1859)	1:79:B:ILE:HG21	1:78:B:LYS:HG2	20	0.37	0.07	0.36
(1,1859)	1:79:B:ILE:HG23	1:78:B:LYS:HG2	20	0.37	0.07	0.36
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	20	0.37	0.07	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1859)	1:79:B:ILE:HG22	1:78:B:LYS:HG2	20	0.37	0.07	0.36
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	20	0.37	0.05	0.36
(1,2574)	1:5:B:THR:HG23	1:83:B:PRO:HG3	20	0.37	0.05	0.36
(1,2574)	1:5:B:THR:HG21	1:83:B:PRO:HG3	20	0.37	0.05	0.36
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	20	0.36	0.13	0.32
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	20	0.36	0.13	0.32
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG21	20	0.36	0.13	0.32
(1,475)	1:79:A:ILE:HG22	1:78:A:LYS:HG2	20	0.36	0.07	0.36
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	20	0.36	0.07	0.36
(1,475)	1:79:A:ILE:HG23	1:78:A:LYS:HG2	20	0.36	0.07	0.36
(1,475)	1:79:A:ILE:HG21	1:78:A:LYS:HG2	20	0.36	0.07	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	20	0.36	0.01	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	20	0.36	0.01	0.36
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	20	0.36	0.08	0.38
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	20	0.36	0.02	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	20	0.36	0.02	0.36
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	20	0.36	0.05	0.37
(1,1693)	1:57:B:THR:HG1	1:58:B:ILE:HA	20	0.36	0.05	0.37
(1,1693)	1:57:B:THR:HG21	1:58:B:ILE:HA	20	0.36	0.05	0.37
(1,1693)	1:57:B:THR:HG22	1:58:B:ILE:HA	20	0.36	0.05	0.37
(1,564)	1:87:A:LEU:HD13	1:60:A:ILE:HG23	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD11	1:60:A:ILE:HG21	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG21	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD12	1:60:A:ILE:HG21	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD23	1:60:A:ILE:HG21	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD23	1:60:A:ILE:HG23	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG23	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD12	1:60:A:ILE:HG23	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG12	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD22	1:60:A:ILE:HG21	20	0.32	0.12	0.28
(1,564)	1:87:A:LEU:HD13	1:60:A:ILE:HG21	20	0.32	0.12	0.28
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	20	0.32	0.04	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	20	0.32	0.04	0.32
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	20	0.32	0.03	0.32
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	20	0.32	0.03	0.32
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	20	0.31	0.03	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	20	0.31	0.03	0.3
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	20	0.31	0.02	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	20	0.31	0.02	0.31
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	20	0.3	0.03	0.3
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	20	0.3	0.03	0.3
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	20	0.28	0.03	0.29

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	20	0.28	0.03	0.29
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	20	0.28	0.01	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	20	0.28	0.01	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	20	0.28	0.01	0.28
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	20	0.28	0.02	0.28
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	20	0.28	0.02	0.28
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	20	0.28	0.02	0.28
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	20	0.27	0.05	0.27
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	20	0.27	0.05	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	20	0.27	0.03	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	20	0.27	0.03	0.27
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	20	0.26	0.02	0.26
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	20	0.26	0.02	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	20	0.26	0.04	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	20	0.26	0.04	0.26
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	20	0.26	0.03	0.25
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	20	0.26	0.03	0.25
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	20	0.26	0.01	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	20	0.26	0.01	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	20	0.26	0.01	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	20	0.26	0.01	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	20	0.26	0.01	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	20	0.26	0.01	0.26
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	20	0.25	0.03	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	20	0.25	0.03	0.25
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	20	0.25	0.02	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	20	0.25	0.02	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	20	0.25	0.02	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	20	0.25	0.02	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	20	0.25	0.02	0.26
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	20	0.25	0.02	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	20	0.25	0.03	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	20	0.25	0.03	0.26
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	20	0.25	0.04	0.25
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	20	0.25	0.04	0.25
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	20	0.25	0.04	0.25
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	20	0.25	0.04	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	20	0.25	0.02	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	20	0.25	0.02	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	20	0.25	0.02	0.25
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	20	0.25	0.06	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	20	0.25	0.06	0.27
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	20	0.24	0.02	0.24
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	20	0.24	0.02	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	20	0.24	0.02	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	20	0.24	0.02	0.24
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	20	0.24	0.03	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	20	0.24	0.03	0.23
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	20	0.24	0.0	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	20	0.24	0.0	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	20	0.24	0.0	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	20	0.24	0.0	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	20	0.24	0.0	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	20	0.24	0.0	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	20	0.24	0.0	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	20	0.24	0.0	0.24
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	20	0.24	0.04	0.24
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	20	0.24	0.04	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	20	0.24	0.0	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	20	0.24	0.0	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	20	0.24	0.0	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	20	0.24	0.0	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	20	0.24	0.0	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	20	0.24	0.0	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	20	0.24	0.0	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	20	0.24	0.0	0.24
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	20	0.24	0.05	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	20	0.24	0.05	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	20	0.24	0.05	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	20	0.24	0.05	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	20	0.24	0.05	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	20	0.24	0.05	0.23
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	20	0.23	0.03	0.24
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	20	0.23	0.04	0.23
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	20	0.23	0.04	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	20	0.23	0.0	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	20	0.23	0.0	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	20	0.23	0.0	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	20	0.23	0.0	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	20	0.23	0.0	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	20	0.23	0.0	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	20	0.23	0.0	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	20	0.23	0.0	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	20	0.23	0.0	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	20	0.23	0.0	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	20	0.23	0.0	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	20	0.23	0.0	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	20	0.23	0.0	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	20	0.23	0.0	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	20	0.23	0.0	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	20	0.23	0.0	0.23
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	20	0.23	0.02	0.24
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	20	0.23	0.02	0.24
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	20	0.23	0.0	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	20	0.23	0.0	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	20	0.23	0.0	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	20	0.23	0.0	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	20	0.23	0.0	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	20	0.23	0.0	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	20	0.23	0.0	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	20	0.23	0.0	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	20	0.23	0.0	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	20	0.23	0.0	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	20	0.23	0.0	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	20	0.23	0.0	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	20	0.23	0.0	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	20	0.23	0.0	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	20	0.23	0.0	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	20	0.23	0.0	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	20	0.23	0.0	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	20	0.23	0.0	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	20	0.23	0.0	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	20	0.23	0.0	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	20	0.23	0.0	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	20	0.23	0.0	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	20	0.23	0.0	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	20	0.23	0.0	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	20	0.23	0.0	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	20	0.23	0.0	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	20	0.23	0.0	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	20	0.23	0.0	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	20	0.23	0.0	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	20	0.23	0.0	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	20	0.23	0.0	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	20	0.23	0.0	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	20	0.23	0.0	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	20	0.23	0.0	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	20	0.23	0.0	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	20	0.23	0.0	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	20	0.23	0.0	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	20	0.23	0.0	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	20	0.23	0.0	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	20	0.23	0.0	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	20	0.23	0.0	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	20	0.23	0.0	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	20	0.23	0.0	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	20	0.23	0.0	0.23
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	20	0.23	0.04	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	20	0.23	0.04	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	20	0.23	0.04	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	20	0.23	0.04	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	20	0.23	0.04	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	20	0.23	0.04	0.24
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	20	0.23	0.0	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	20	0.23	0.0	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	20	0.23	0.0	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	20	0.23	0.0	0.23
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	20	0.22	0.0	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	20	0.22	0.0	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	20	0.22	0.0	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	20	0.22	0.0	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	20	0.22	0.0	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	20	0.22	0.0	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	20	0.22	0.0	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	20	0.22	0.0	0.22
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	20	0.22	0.03	0.22
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	20	0.22	0.03	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	20	0.22	0.0	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	20	0.22	0.0	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	20	0.22	0.0	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	20	0.22	0.0	0.22
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	20	0.22	0.03	0.21
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	20	0.22	0.0	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	20	0.22	0.0	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	20	0.22	0.0	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	20	0.22	0.0	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	20	0.22	0.0	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	20	0.22	0.0	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	20	0.22	0.0	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	20	0.22	0.0	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	20	0.22	0.0	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	20	0.22	0.0	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	20	0.22	0.0	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	20	0.22	0.0	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	20	0.22	0.0	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	20	0.22	0.0	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	20	0.22	0.0	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	20	0.22	0.0	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	20	0.22	0.0	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	20	0.22	0.0	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	20	0.22	0.0	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	20	0.22	0.0	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	20	0.22	0.0	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	20	0.22	0.0	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	20	0.22	0.0	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	20	0.22	0.0	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	20	0.22	0.0	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	20	0.22	0.0	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	20	0.22	0.0	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	20	0.22	0.0	0.22
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	20	0.22	0.06	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	20	0.22	0.06	0.22
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	20	0.22	0.03	0.22
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	20	0.22	0.03	0.22
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	20	0.21	0.02	0.22
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	20	0.21	0.02	0.22
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	20	0.21	0.03	0.21
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	20	0.21	0.03	0.21
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	20	0.21	0.02	0.22
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	20	0.21	0.02	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	20	0.21	0.01	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	20	0.21	0.01	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	20	0.21	0.01	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	20	0.21	0.01	0.21
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	20	0.21	0.02	0.21
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	20	0.21	0.02	0.21
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	20	0.21	0.06	0.2
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	20	0.19	0.03	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	20	0.19	0.03	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	20	0.19	0.02	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	20	0.19	0.02	0.18
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	20	0.18	0.03	0.19
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	20	0.18	0.03	0.19
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	20	0.18	0.04	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	20	0.18	0.04	0.17
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	20	0.18	0.03	0.18
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	20	0.18	0.04	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	20	0.18	0.02	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	20	0.18	0.02	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	20	0.18	0.02	0.18
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	20	0.18	0.03	0.18
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	20	0.18	0.03	0.18
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	20	0.18	0.03	0.18
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	20	0.18	0.03	0.18
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	20	0.18	0.02	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	20	0.18	0.03	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	20	0.18	0.03	0.18
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	20	0.17	0.03	0.16
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	20	0.17	0.03	0.16
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	20	0.17	0.03	0.16
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	20	0.16	0.02	0.16
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	20	0.16	0.02	0.16
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	20	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	20	0.16	0.03	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	20	0.16	0.03	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	20	0.15	0.02	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	20	0.15	0.02	0.15
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	20	0.15	0.03	0.14
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	20	0.15	0.03	0.14
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	20	0.15	0.02	0.15
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	20	0.15	0.02	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	20	0.15	0.02	0.15
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	20	0.15	0.02	0.15
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	20	0.14	0.02	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	20	0.14	0.02	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	20	0.14	0.02	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	20	0.14	0.01	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	20	0.14	0.01	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	20	0.13	0.02	0.13
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	20	0.13	0.02	0.13
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	19	0.63	0.19	0.55
(1,1971)	1:60:B:ILE:HG21	1:90:B:PHE:HZ	19	0.63	0.19	0.55
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG13	19	0.63	0.29	0.71
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	19	0.63	0.29	0.71
(1,1928)	1:85:B:ASN:HB2	1:60:B:ILE:HG23	19	0.63	0.29	0.71
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG22	19	0.63	0.29	0.71
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG12	19	0.63	0.29	0.71
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG21	19	0.63	0.29	0.71
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	19	0.55	0.25	0.55
(1,302)	1:57:A:THR:HG23	1:43:A:ILE:HB	19	0.55	0.25	0.55
(1,302)	1:57:A:THR:HG21	1:43:A:ILE:HB	19	0.55	0.25	0.55
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	19	0.48	0.1	0.48
(1,361)	1:43:A:ILE:HG21	1:65:A:PHE:HB3	19	0.48	0.1	0.48
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	19	0.38	0.2	0.34
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG21	19	0.38	0.2	0.34
(1,726)	1:101:A:LEU:HB2	1:102:A:ILE:HG21	19	0.38	0.2	0.34
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG21	19	0.36	0.17	0.34
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	19	0.36	0.17	0.34
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	19	0.36	0.17	0.34
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG1	19	0.36	0.17	0.34
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	19	0.34	0.08	0.36
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG21	19	0.29	0.09	0.27
(1,1948)	1:87:B:LEU:HD13	1:60:B:ILE:HG23	19	0.29	0.09	0.27
(1,1948)	1:87:B:LEU:HD21	1:60:B:ILE:HG21	19	0.29	0.09	0.27
(1,1948)	1:87:B:LEU:HD13	1:60:B:ILE:HG21	19	0.29	0.09	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG23	19	0.29	0.09	0.27
(1,1948)	1:87:B:LEU:HD11	1:60:B:ILE:HG23	19	0.29	0.09	0.27
(1,1948)	1:87:B:LEU:HD21	1:60:B:ILE:HG23	19	0.29	0.09	0.27
(1,1948)	1:87:B:LEU:HD22	1:60:B:ILE:HG21	19	0.29	0.09	0.27
(1,1948)	1:87:B:LEU:HD12	1:60:B:ILE:HG21	19	0.29	0.09	0.27
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	19	0.23	0.07	0.24
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	19	0.23	0.07	0.24
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	19	0.23	0.07	0.24
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	19	0.23	0.07	0.24
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	19	0.17	0.04	0.16
(1,420)	1:73:A:THR:HG23	1:39:A:PRO:HG3	19	0.17	0.04	0.16
(1,420)	1:73:A:THR:HG1	1:39:A:PRO:HG3	19	0.17	0.04	0.16
(1,420)	1:73:A:THR:HG21	1:39:A:PRO:HG3	19	0.17	0.04	0.16
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	19	0.14	0.02	0.14
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	19	0.14	0.02	0.14
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD13	18	0.73	0.32	0.82
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD13	18	0.73	0.32	0.82
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD12	18	0.73	0.32	0.82
(1,1711)	1:60:B:ILE:HG22	1:58:B:ILE:HD11	18	0.73	0.32	0.82
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD11	18	0.73	0.32	0.82
(1,1711)	1:60:B:ILE:HG13	1:58:B:ILE:HD11	18	0.73	0.32	0.82
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD12	18	0.73	0.32	0.82
(1,1711)	1:60:B:ILE:HG22	1:58:B:ILE:HD12	18	0.73	0.32	0.82
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG21	18	0.43	0.15	0.4
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG21	18	0.43	0.15	0.4
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG12	18	0.43	0.15	0.4
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG13	18	0.43	0.15	0.4
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG13	18	0.43	0.15	0.4
(1,723)	1:98:A:ILE:HD11	1:102:A:ILE:HG12	18	0.43	0.15	0.4
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG12	18	0.43	0.15	0.4
(1,723)	1:98:A:ILE:HD11	1:102:A:ILE:HG13	18	0.43	0.15	0.4
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG21	18	0.4	0.07	0.38
(1,2107)	1:98:B:ILE:HD13	1:102:B:ILE:HG13	18	0.4	0.07	0.38
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG13	18	0.4	0.07	0.38
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG21	18	0.4	0.07	0.38
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG13	18	0.4	0.07	0.38
(1,2107)	1:98:B:ILE:HD13	1:102:B:ILE:HG21	18	0.4	0.07	0.38
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG12	18	0.4	0.07	0.38
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD13	18	0.39	0.13	0.37
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD12	18	0.39	0.13	0.37
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	18	0.39	0.13	0.37
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	18	0.32	0.04	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	18	0.32	0.04	0.32
(1,1048)	1:41:A:THR:HG22	1:66:A:ILE:HB	18	0.3	0.07	0.31
(1,1048)	1:41:A:THR:HG21	1:66:A:ILE:HB	18	0.3	0.07	0.31
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	18	0.3	0.07	0.31
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	18	0.29	0.02	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	18	0.29	0.02	0.3
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	18	0.23	0.04	0.24
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	18	0.16	0.04	0.16
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	18	0.16	0.04	0.16
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	18	0.16	0.03	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	18	0.16	0.03	0.15
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	18	0.15	0.04	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	18	0.15	0.04	0.13
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	18	0.15	0.02	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	18	0.15	0.02	0.14
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	18	0.14	0.02	0.13
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	18	0.14	0.02	0.13
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	18	0.13	0.02	0.13
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	18	0.13	0.02	0.12
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	18	0.12	0.01	0.12
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	18	0.12	0.01	0.12
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD13	17	0.71	0.31	0.79

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD13	17	0.71	0.31	0.79
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD11	17	0.71	0.31	0.79
(1,327)	1:60:A:ILE:HG22	1:58:A:ILE:HD12	17	0.71	0.31	0.79
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD12	17	0.71	0.31	0.79
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD12	17	0.71	0.31	0.79
(1,327)	1:60:A:ILE:HG13	1:58:A:ILE:HD12	17	0.71	0.31	0.79
(1,327)	1:60:A:ILE:HG22	1:58:A:ILE:HD11	17	0.71	0.31	0.79
(1,2114)	1:103:B:THR:HG23	1:99:B:ASP:HB2	17	0.62	0.32	0.46
(1,2114)	1:103:B:THR:HG21	1:99:B:ASP:HB2	17	0.62	0.32	0.46
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB2	17	0.62	0.32	0.46
(1,2114)	1:103:B:THR:HG21	1:99:B:ASP:HB3	17	0.62	0.32	0.46
(1,2114)	1:103:B:THR:HG22	1:99:B:ASP:HB2	17	0.62	0.32	0.46
(1,2114)	1:103:B:THR:HG22	1:99:B:ASP:HB3	17	0.62	0.32	0.46
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB3	17	0.62	0.32	0.46
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG23	17	0.43	0.16	0.44
(1,421)	1:71:A:GLN:HB2	1:73:A:THR:HG23	17	0.43	0.16	0.44
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	17	0.43	0.16	0.44
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG21	17	0.43	0.16	0.44
(1,421)	1:71:A:GLN:HB2	1:73:A:THR:HG21	17	0.43	0.16	0.44
(1,421)	1:71:A:GLN:HB2	1:73:A:THR:HG22	17	0.43	0.16	0.44
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG23	17	0.41	0.12	0.38
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG21	17	0.41	0.12	0.38
(1,1805)	1:71:B:GLN:HB2	1:73:B:THR:HG22	17	0.41	0.12	0.38
(1,1805)	1:71:B:GLN:HB2	1:73:B:THR:HG23	17	0.41	0.12	0.38
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG1	17	0.41	0.12	0.38
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG22	17	0.41	0.12	0.38
(1,2053)	1:69:B:THR:HG1	1:98:B:ILE:H	17	0.32	0.15	0.26
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	17	0.32	0.15	0.26
(1,2053)	1:69:B:THR:HG21	1:98:B:ILE:H	17	0.32	0.15	0.26
(1,2053)	1:69:B:THR:HG22	1:98:B:ILE:H	17	0.32	0.15	0.26
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	17	0.29	0.07	0.27
(1,2432)	1:41:B:THR:HG21	1:66:B:ILE:HB	17	0.29	0.07	0.27
(1,2432)	1:41:B:THR:HG22	1:66:B:ILE:HB	17	0.29	0.07	0.27
(1,1804)	1:73:B:THR:HG23	1:39:B:PRO:HG3	17	0.18	0.07	0.18
(1,1804)	1:73:B:THR:HG21	1:39:B:PRO:HG3	17	0.18	0.07	0.18
(1,1804)	1:73:B:THR:HG22	1:39:B:PRO:HG3	17	0.18	0.07	0.18
(1,1804)	1:73:B:THR:HG1	1:39:B:PRO:HG3	17	0.18	0.07	0.18
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	17	0.14	0.02	0.14
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	17	0.14	0.02	0.14
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	17	0.13	0.02	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	17	0.13	0.02	0.13
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	17	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	17	0.13	0.02	0.13
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	17	0.13	0.02	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG21	17	0.13	0.02	0.14
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	17	0.12	0.02	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	17	0.12	0.02	0.13
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	17	0.12	0.01	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	17	0.12	0.01	0.12
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	16	0.62	0.3	0.58
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	16	0.62	0.3	0.58
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	16	0.56	0.19	0.6
(1,1686)	1:57:B:THR:HG21	1:43:B:ILE:HB	16	0.56	0.19	0.6
(1,1686)	1:57:B:THR:HG23	1:43:B:ILE:HB	16	0.56	0.19	0.6
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB3	16	0.49	0.29	0.4
(1,730)	1:103:A:THR:HG22	1:99:A:ASP:HB2	16	0.49	0.29	0.4
(1,730)	1:103:A:THR:HG21	1:99:A:ASP:HB2	16	0.49	0.29	0.4
(1,730)	1:103:A:THR:HG21	1:99:A:ASP:HB3	16	0.49	0.29	0.4
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB2	16	0.49	0.29	0.4
(1,730)	1:103:A:THR:HG23	1:99:A:ASP:HB2	16	0.49	0.29	0.4
(1,730)	1:103:A:THR:HG22	1:99:A:ASP:HB3	16	0.49	0.29	0.4
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD2	16	0.38	0.09	0.36
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	16	0.38	0.09	0.36
(1,594)	1:89:A:THR:HG21	1:90:A:PHE:HB2	16	0.24	0.05	0.24
(1,594)	1:89:A:THR:HG23	1:90:A:PHE:HB2	16	0.24	0.05	0.24
(1,594)	1:89:A:THR:HG1	1:90:A:PHE:HB2	16	0.24	0.05	0.24
(1,594)	1:89:A:THR:HG22	1:90:A:PHE:HB2	16	0.24	0.05	0.24
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	16	0.21	0.08	0.2
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	16	0.21	0.08	0.2
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	16	0.13	0.05	0.12
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	15	1.12	0.28	1.19
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG12	15	1.12	0.28	1.19
(1,647)	1:93:A:GLU:HG3	1:94:A:ILE:HG13	15	1.12	0.28	1.19
(1,2758)	1:103:B:THR:HG23	1:102:B:ILE:HG23	15	0.6	0.24	0.62
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	15	0.6	0.24	0.62
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG22	15	0.6	0.24	0.62
(1,2758)	1:103:B:THR:HG21	1:102:B:ILE:HG22	15	0.6	0.24	0.62
(1,2758)	1:103:B:THR:HG22	1:102:B:ILE:HG12	15	0.6	0.24	0.62
(1,2758)	1:103:B:THR:HG22	1:102:B:ILE:HG23	15	0.6	0.24	0.62
(1,2758)	1:103:B:THR:HG21	1:102:B:ILE:HG23	15	0.6	0.24	0.62
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD12	15	0.48	0.15	0.43
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD11	15	0.48	0.15	0.43
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD13	15	0.48	0.15	0.43
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	15	0.43	0.13	0.41

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1745)	1:43:B:ILE:HG12	1:65:B:PHE:HB3	15	0.43	0.13	0.41
(1,1745)	1:43:B:ILE:HG21	1:65:B:PHE:HB3	15	0.43	0.13	0.41
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG22	15	0.38	0.1	0.36
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG21	15	0.38	0.1	0.36
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	15	0.38	0.1	0.36
(1,1978)	1:89:B:THR:HG21	1:90:B:PHE:HB2	15	0.22	0.05	0.22
(1,1978)	1:89:B:THR:HG23	1:90:B:PHE:HB2	15	0.22	0.05	0.22
(1,1978)	1:89:B:THR:HG1	1:90:B:PHE:HB2	15	0.22	0.05	0.22
(1,1978)	1:89:B:THR:HG22	1:90:B:PHE:HB2	15	0.22	0.05	0.22
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	15	0.18	0.04	0.17
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	15	0.13	0.02	0.13
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	15	0.13	0.02	0.13
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	15	0.12	0.01	0.12
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	15	0.12	0.01	0.12
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	15	0.12	0.01	0.12
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	15	0.12	0.01	0.12
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	15	0.12	0.01	0.12
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	15	0.12	0.01	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	15	0.12	0.01	0.12
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	14	0.61	0.22	0.57
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG21	14	0.61	0.22	0.57
(1,544)	1:85:A:ASN:HB2	1:60:A:ILE:HG23	14	0.61	0.22	0.57
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	14	0.15	0.02	0.15
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	14	0.15	0.02	0.15
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	14	0.15	0.02	0.15
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	14	0.14	0.02	0.14
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	14	0.14	0.02	0.14
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	14	0.14	0.06	0.12
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	14	0.13	0.02	0.13
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	14	0.13	0.02	0.13
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	14	0.13	0.02	0.13
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	14	0.13	0.02	0.13
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	14	0.13	0.02	0.13
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	14	0.13	0.02	0.13
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	14	0.13	0.02	0.12
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	14	0.13	0.02	0.12
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	14	0.13	0.01	0.13
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	14	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	14	0.13	0.02	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	14	0.13	0.02	0.12
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	14	0.12	0.01	0.12
(1,1374)	1:103:A:THR:HG21	1:102:A:ILE:HG23	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG23	1:102:A:ILE:HG23	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG23	1:102:A:ILE:HG12	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG23	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG21	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG21	1:102:A:ILE:HG13	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG12	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG22	1:102:A:ILE:HG23	13	0.61	0.29	0.68
(1,1374)	1:103:A:THR:HG22	1:102:A:ILE:HG13	13	0.61	0.29	0.68
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	13	0.4	0.15	0.31
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD2	13	0.4	0.15	0.31
(1,669)	1:69:A:THR:HG1	1:98:A:ILE:H	13	0.37	0.11	0.43
(1,669)	1:69:A:THR:HG22	1:98:A:ILE:H	13	0.37	0.11	0.43
(1,669)	1:69:A:THR:HG23	1:98:A:ILE:H	13	0.37	0.11	0.43
(1,669)	1:69:A:THR:HG21	1:98:A:ILE:H	13	0.37	0.11	0.43
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	13	0.24	0.04	0.24
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	13	0.21	0.13	0.16
(1,409)	1:69:A:THR:HG23	1:54:A:LEU:HA	13	0.21	0.13	0.16
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	13	0.21	0.05	0.22
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	13	0.21	0.05	0.22
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	13	0.21	0.05	0.22
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	13	0.17	0.06	0.14
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG21	13	0.14	0.02	0.14
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	13	0.14	0.02	0.14
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	13	0.14	0.03	0.12
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	13	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	13	0.12	0.02	0.12
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	13	0.12	0.02	0.12
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	12	0.64	0.13	0.64
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB2	12	0.55	0.24	0.53
(1,2413)	1:43:B:ILE:HG22	1:64:B:ASP:HB2	12	0.55	0.24	0.53
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	12	0.55	0.24	0.53
(1,2413)	1:43:B:ILE:HG22	1:64:B:ASP:HB3	12	0.55	0.24	0.53
(1,416)	1:37:A:VAL:HG23	1:73:A:THR:HG21	12	0.43	0.13	0.42
(1,416)	1:37:A:VAL:HG22	1:73:A:THR:HG1	12	0.43	0.13	0.42
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG21	12	0.43	0.13	0.42
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG22	12	0.43	0.13	0.42
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG1	12	0.43	0.13	0.42
(1,416)	1:37:A:VAL:HG22	1:73:A:THR:HG23	12	0.43	0.13	0.42
(1,1959)	1:89:B:THR:HG21	1:87:B:LEU:HB2	12	0.42	0.21	0.46
(1,1959)	1:89:B:THR:HG23	1:87:B:LEU:HB2	12	0.42	0.21	0.46
(1,1959)	1:89:B:THR:HG1	1:87:B:LEU:HB2	12	0.42	0.21	0.46
(1,1959)	1:89:B:THR:HG22	1:87:B:LEU:HB2	12	0.42	0.21	0.46
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG22	12	0.36	0.13	0.37
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG21	12	0.36	0.13	0.37
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG23	12	0.36	0.13	0.37
(1,410)	1:69:A:THR:HG22	1:56:A:PRO:HD3	12	0.36	0.17	0.32
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	12	0.36	0.17	0.32
(1,410)	1:69:A:THR:HG23	1:56:A:PRO:HD3	12	0.36	0.17	0.32
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD2	12	0.36	0.17	0.32
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	12	0.26	0.11	0.32
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	12	0.26	0.11	0.32
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	12	0.26	0.11	0.32
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	12	0.25	0.13	0.24
(1,1380)	1:103:A:THR:HG21	1:105:A:ILE:HB	12	0.25	0.13	0.24
(1,1380)	1:103:A:THR:HG23	1:105:A:ILE:HB	12	0.25	0.13	0.24
(1,1380)	1:103:A:THR:HG22	1:105:A:ILE:HB	12	0.25	0.13	0.24
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	12	0.24	0.08	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	12	0.24	0.08	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	12	0.24	0.08	0.28
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	12	0.22	0.05	0.22
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	12	0.22	0.05	0.22
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	12	0.22	0.05	0.22
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	12	0.22	0.05	0.22
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	12	0.22	0.05	0.22
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	12	0.22	0.05	0.22
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	12	0.19	0.05	0.22
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	12	0.19	0.05	0.22
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	12	0.19	0.05	0.22
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	12	0.13	0.03	0.12
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	11	0.67	0.06	0.66
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG21	11	0.65	0.2	0.71
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG1	11	0.65	0.2	0.71
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG22	11	0.65	0.2	0.71
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG23	11	0.65	0.2	0.71

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG23	11	0.5	0.23	0.53
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG22	11	0.5	0.23	0.53
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG13	11	0.5	0.23	0.53
(1,417)	1:37:A:VAL:HG23	1:73:A:THR:HG21	11	0.29	0.1	0.28
(1,417)	1:37:A:VAL:HG22	1:73:A:THR:HG1	11	0.29	0.1	0.28
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG21	11	0.29	0.1	0.28
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG22	11	0.29	0.1	0.28
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG1	11	0.29	0.1	0.28
(1,417)	1:37:A:VAL:HG22	1:73:A:THR:HG23	11	0.29	0.1	0.28
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	11	0.29	0.07	0.31
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	11	0.29	0.07	0.31
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	11	0.28	0.09	0.31
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	11	0.28	0.09	0.31
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	11	0.28	0.09	0.31
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	11	0.23	0.07	0.26
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	11	0.23	0.07	0.26
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	11	0.23	0.07	0.26
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	11	0.23	0.07	0.26
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	11	0.23	0.07	0.26
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	11	0.23	0.07	0.26
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	11	0.15	0.02	0.14
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	11	0.15	0.02	0.14
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	11	0.14	0.02	0.14
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	11	0.14	0.02	0.14
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	11	0.13	0.02	0.14
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	11	0.12	0.01	0.13
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	11	0.12	0.01	0.13
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	11	0.11	0.01	0.11
(1,341)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	10	0.46	0.23	0.46
(1,341)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	10	0.46	0.23	0.46
(1,187)	1:34:A:THR:HG22	1:34:A:THR:HA	10	0.42	0.04	0.42
(1,187)	1:34:A:THR:HG21	1:34:A:THR:HA	10	0.42	0.04	0.42
(1,187)	1:34:A:THR:HG23	1:34:A:THR:HA	10	0.42	0.04	0.42
(1,575)	1:89:A:THR:HG23	1:87:A:LEU:HB2	10	0.35	0.17	0.31
(1,575)	1:89:A:THR:HG22	1:87:A:LEU:HB2	10	0.35	0.17	0.31
(1,575)	1:89:A:THR:HG21	1:87:A:LEU:HB2	10	0.35	0.17	0.31
(1,575)	1:89:A:THR:HG1	1:87:A:LEU:HB2	10	0.35	0.17	0.31
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	10	0.25	0.03	0.24
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	10	0.25	0.03	0.24
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	10	0.23	0.07	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	10	0.23	0.07	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	10	0.23	0.07	0.28
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	10	0.22	0.05	0.21
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	10	0.22	0.05	0.21
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	10	0.22	0.05	0.21
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	10	0.22	0.05	0.21
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	10	0.22	0.05	0.21
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	10	0.22	0.05	0.21
(1,2764)	1:103:B:THR:HG1	1:105:B:ILE:HB	10	0.22	0.05	0.23
(1,2764)	1:103:B:THR:HG21	1:105:B:ILE:HB	10	0.22	0.05	0.23
(1,2764)	1:103:B:THR:HG22	1:105:B:ILE:HB	10	0.22	0.05	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2764)	1:103:B:THR:HG23	1:105:B:ILE:HB	10	0.22	0.05	0.23
(1,278)	1:48:A:LYS:HD3	1:43:A:ILE:HG21	10	0.17	0.06	0.13
(1,278)	1:48:A:LYS:HD2	1:43:A:ILE:HG21	10	0.17	0.06	0.13
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	10	0.15	0.05	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	10	0.15	0.05	0.12
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	10	0.14	0.02	0.14
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	10	0.14	0.02	0.14
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	10	0.12	0.02	0.12
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	10	0.12	0.02	0.12
(1,338)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	9	0.46	0.2	0.57
(1,338)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	9	0.46	0.2	0.57
(1,311)	1:58:A:ILE:HG12	1:57:A:THR:HB	9	0.27	0.12	0.26
(1,311)	1:58:A:ILE:HG13	1:57:A:THR:HB	9	0.27	0.12	0.26
(1,311)	1:58:A:ILE:HG21	1:57:A:THR:HB	9	0.27	0.12	0.26
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	9	0.24	0.07	0.25
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	9	0.24	0.07	0.25
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	9	0.24	0.07	0.25
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	9	0.24	0.07	0.25
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	9	0.24	0.07	0.25
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	9	0.24	0.07	0.25
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	9	0.23	0.04	0.25
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	9	0.23	0.04	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	9	0.2	0.09	0.18
(1,2121)	1:105:B:ILE:HG21	1:99:B:ASP:HA	9	0.2	0.09	0.18
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	9	0.14	0.02	0.14
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	9	0.14	0.02	0.14
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	9	0.13	0.02	0.13
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	9	0.13	0.02	0.13
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	9	0.13	0.02	0.13
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	9	0.13	0.03	0.12
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	9	0.13	0.02	0.13
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	9	0.13	0.02	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	9	0.12	0.0	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	9	0.12	0.0	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	9	0.12	0.0	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	9	0.12	0.0	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	9	0.12	0.0	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	9	0.12	0.0	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	9	0.12	0.0	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	9	0.12	0.0	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	9	0.12	0.01	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	9	0.12	0.01	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	9	0.12	0.01	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	9	0.12	0.01	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	9	0.12	0.01	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	9	0.12	0.01	0.12
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	9	0.11	0.01	0.11
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	8	0.42	0.2	0.38
(1,689)	1:69:A:THR:HG21	1:100:A:PHE:HD2	8	0.42	0.2	0.38
(1,1571)	1:34:B:THR:HG1	1:34:B:THR:HA	8	0.39	0.06	0.38
(1,1571)	1:34:B:THR:HG21	1:34:B:THR:HA	8	0.39	0.06	0.38
(1,1571)	1:34:B:THR:HG22	1:34:B:THR:HA	8	0.39	0.06	0.38
(1,1571)	1:34:B:THR:HG23	1:34:B:THR:HA	8	0.39	0.06	0.38
(1,1725)	1:64:B:ASP:HB2	1:43:B:ILE:HG13	8	0.35	0.18	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1725)	1:64:B:ASP:HB2	1:43:B:ILE:HG22	8	0.35	0.18	0.27
(1,1725)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	8	0.35	0.18	0.27
(1,1794)	1:69:B:THR:HG1	1:56:B:PRO:HD3	8	0.32	0.08	0.3
(1,1794)	1:69:B:THR:HG22	1:56:B:PRO:HD3	8	0.32	0.08	0.3
(1,1794)	1:69:B:THR:HG23	1:56:B:PRO:HD3	8	0.32	0.08	0.3
(1,1722)	1:64:B:ASP:HB2	1:43:B:ILE:HG13	8	0.31	0.18	0.23
(1,1722)	1:64:B:ASP:HB2	1:43:B:ILE:HG22	8	0.31	0.18	0.23
(1,1722)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	8	0.31	0.18	0.23
(1,1695)	1:58:B:ILE:HG13	1:57:B:THR:HB	8	0.31	0.08	0.29
(1,1695)	1:58:B:ILE:HG12	1:57:B:THR:HB	8	0.31	0.08	0.29
(1,1695)	1:58:B:ILE:HG21	1:57:B:THR:HB	8	0.31	0.08	0.29
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	8	0.28	0.09	0.28
(1,737)	1:105:A:ILE:HG12	1:99:A:ASP:HA	8	0.28	0.09	0.28
(1,581)	1:58:A:ILE:HG21	1:90:A:PHE:HD1	8	0.24	0.07	0.23
(1,581)	1:58:A:ILE:HG23	1:90:A:PHE:HD2	8	0.24	0.07	0.23
(1,581)	1:58:A:ILE:HG22	1:90:A:PHE:HD2	8	0.24	0.07	0.23
(1,581)	1:58:A:ILE:HG23	1:90:A:PHE:HD1	8	0.24	0.07	0.23
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	8	0.15	0.02	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	8	0.15	0.02	0.16
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	8	0.13	0.02	0.12
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	8	0.13	0.02	0.12
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	8	0.12	0.02	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	8	0.12	0.02	0.11
(1,2376)	1:58:B:ILE:HG13	1:56:B:PRO:HB2	7	0.28	0.12	0.25
(1,2376)	1:58:B:ILE:HG23	1:56:B:PRO:HB2	7	0.28	0.12	0.25
(1,2376)	1:58:B:ILE:HG21	1:56:B:PRO:HB2	7	0.28	0.12	0.25
(1,2376)	1:58:B:ILE:HG12	1:56:B:PRO:HB2	7	0.28	0.12	0.25
(1,1793)	1:69:B:THR:HG1	1:54:B:LEU:HA	7	0.26	0.12	0.22
(1,1793)	1:69:B:THR:HG22	1:54:B:LEU:HA	7	0.26	0.12	0.22
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG13	7	0.26	0.13	0.23
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG23	7	0.26	0.13	0.23
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG21	7	0.26	0.13	0.23

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG12	7	0.26	0.13	0.23
(1,733)	1:103:A:THR:HG22	1:102:A:ILE:HB	7	0.23	0.04	0.25
(1,733)	1:103:A:THR:HG21	1:102:A:ILE:HB	7	0.23	0.04	0.25
(1,733)	1:103:A:THR:HG23	1:102:A:ILE:HB	7	0.23	0.04	0.25
(1,733)	1:103:A:THR:HG1	1:102:A:ILE:HB	7	0.23	0.04	0.25
(1,1965)	1:58:B:ILE:HG21	1:90:B:PHE:HD2	7	0.2	0.08	0.18
(1,1965)	1:58:B:ILE:HG21	1:90:B:PHE:HD1	7	0.2	0.08	0.18
(1,1965)	1:58:B:ILE:HG13	1:90:B:PHE:HD2	7	0.2	0.08	0.18
(1,1965)	1:58:B:ILE:HG23	1:90:B:PHE:HD2	7	0.2	0.08	0.18
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD13	7	0.17	0.08	0.15
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD21	7	0.17	0.08	0.15
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD12	7	0.17	0.08	0.15
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD23	7	0.17	0.08	0.15
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG22	7	0.14	0.02	0.13
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG21	7	0.14	0.02	0.13
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG23	7	0.14	0.02	0.13
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	7	0.14	0.03	0.14
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	7	0.13	0.05	0.12
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	7	0.13	0.05	0.12
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	7	0.13	0.05	0.12
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	7	0.13	0.03	0.14
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	7	0.13	0.03	0.14
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	7	0.13	0.02	0.12
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	7	0.13	0.02	0.12
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	7	0.13	0.02	0.12
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	7	0.13	0.02	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	7	0.12	0.01	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	7	0.12	0.01	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	7	0.12	0.01	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	7	0.12	0.01	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	7	0.12	0.01	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	7	0.12	0.01	0.12
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	7	0.12	0.01	0.12
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	7	0.12	0.02	0.11
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	7	0.12	0.02	0.11
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	7	0.12	0.02	0.11
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	7	0.12	0.02	0.11
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	7	0.12	0.02	0.11
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	7	0.12	0.02	0.11
(1,641)	1:94:A:ILE:HG13	1:22:A:VAL:HB	7	0.12	0.01	0.11
(1,641)	1:94:A:ILE:HG21	1:22:A:VAL:HB	7	0.12	0.01	0.11
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	7	0.11	0.01	0.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG13	6	0.55	0.17	0.49
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG23	6	0.55	0.17	0.49
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG21	6	0.55	0.17	0.49
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG22	6	0.55	0.17	0.49
(1,2085)	1:69:B:THR:HG23	1:101:B:LEU:HB3	6	0.42	0.23	0.36
(1,2085)	1:69:B:THR:HG21	1:101:B:LEU:HB3	6	0.42	0.23	0.36
(1,701)	1:69:A:THR:HG23	1:101:A:LEU:HB3	6	0.31	0.15	0.3
(1,701)	1:69:A:THR:HG21	1:101:A:LEU:HB3	6	0.31	0.15	0.3
(1,701)	1:69:A:THR:HG22	1:101:A:LEU:HB3	6	0.31	0.15	0.3
(1,701)	1:69:A:THR:HG21	1:101:A:LEU:HB2	6	0.31	0.15	0.3
(1,1800)	1:37:B:VAL:HG22	1:73:B:THR:HG22	6	0.27	0.08	0.28
(1,1800)	1:37:B:VAL:HG23	1:73:B:THR:HG22	6	0.27	0.08	0.28
(1,1800)	1:37:B:VAL:HG22	1:73:B:THR:HG23	6	0.27	0.08	0.28
(1,1800)	1:37:B:VAL:HG22	1:73:B:THR:HG1	6	0.27	0.08	0.28
(1,1800)	1:37:B:VAL:HG21	1:73:B:THR:HG21	6	0.27	0.08	0.28
(1,1800)	1:37:B:VAL:HG23	1:73:B:THR:HG1	6	0.27	0.08	0.28
(1,2117)	1:103:B:THR:HG21	1:102:B:ILE:HB	6	0.26	0.01	0.26
(1,2117)	1:103:B:THR:HG23	1:102:B:ILE:HB	6	0.26	0.01	0.26
(1,2117)	1:103:B:THR:HG22	1:102:B:ILE:HB	6	0.26	0.01	0.26
(1,1662)	1:48:B:LYS:HD3	1:43:B:ILE:HG21	6	0.18	0.05	0.17
(1,1662)	1:48:B:LYS:HD2	1:43:B:ILE:HG21	6	0.18	0.05	0.17
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB2	6	0.15	0.05	0.12
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB3	6	0.15	0.05	0.12
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB2	6	0.15	0.05	0.12
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB3	6	0.15	0.05	0.12
(1,1765)	1:66:B:ILE:HG13	1:43:B:ILE:HG21	6	0.14	0.02	0.14
(1,1765)	1:66:B:ILE:HG21	1:43:B:ILE:HG13	6	0.14	0.02	0.14
(1,326)	1:60:A:ILE:HG12	1:58:A:ILE:HG12	6	0.14	0.02	0.15
(1,326)	1:60:A:ILE:HG21	1:58:A:ILE:HG12	6	0.14	0.02	0.15
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG2	6	0.13	0.01	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG3	6	0.13	0.01	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG2	6	0.13	0.01	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG3	6	0.13	0.01	0.13
(1,3052)	1:36:B:LEU:H	1:26:B:SER:H	6	0.13	0.01	0.13
(1,56)	1:9:A:ASN:HB2	1:15:A:ALA:HA	6	0.12	0.02	0.13
(1,56)	1:9:A:ASN:HB3	1:15:A:ALA:HA	6	0.12	0.02	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD11	6	0.12	0.01	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD12	6	0.12	0.01	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD13	6	0.12	0.01	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD21	6	0.12	0.01	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD22	6	0.12	0.01	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD23	6	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1635)	1:19:B:PRO:HG2	1:41:B:THR:HB	6	0.12	0.02	0.12
(1,1635)	1:19:B:PRO:HG3	1:41:B:THR:HB	6	0.12	0.02	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB2	6	0.11	0.01	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB3	6	0.11	0.01	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB2	6	0.11	0.01	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB3	6	0.11	0.01	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB2	6	0.11	0.01	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB3	6	0.11	0.01	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB2	6	0.11	0.01	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB3	6	0.11	0.01	0.12
(1,3141)	1:26:B:SER:H	1:25:B:GLN:HA	6	0.11	0.01	0.11
(1,336)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	5	0.42	0.05	0.44
(1,336)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	5	0.42	0.05	0.44
(1,2073)	1:69:B:THR:HG1	1:100:B:PHE:HD2	5	0.37	0.11	0.37
(1,2073)	1:69:B:THR:HG23	1:100:B:PHE:HD2	5	0.37	0.11	0.37
(1,340)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	5	0.19	0.05	0.21
(1,340)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	5	0.19	0.05	0.21
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD13	5	0.18	0.07	0.16
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD23	5	0.18	0.07	0.16
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD11	5	0.18	0.07	0.16
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD21	5	0.18	0.07	0.16
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG11	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG12	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG13	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG21	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG22	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG23	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG11	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG12	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG13	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG21	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG22	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG23	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG11	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG12	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG13	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG21	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG22	5	0.17	0.06	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG23	5	0.17	0.06	0.15
(1,1450)	1:17:B:THR:HG1	1:16:B:LYS:HB3	5	0.16	0.07	0.14
(1,1450)	1:17:B:THR:HG1	1:16:B:LYS:HB2	5	0.16	0.07	0.14
(1,1450)	1:17:B:THR:HG23	1:16:B:LYS:HB2	5	0.16	0.07	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,343)	1:58:A:ILE:HB	1:64:A:ASP:HA	5	0.14	0.03	0.13
(1,1157)	1:79:A:ILE:HD11	1:75:A:VAL:HB	5	0.14	0.04	0.12
(1,1157)	1:79:A:ILE:HD12	1:75:A:VAL:HB	5	0.14	0.04	0.12
(1,1157)	1:79:A:ILE:HD13	1:75:A:VAL:HB	5	0.14	0.04	0.12
(1,1789)	1:40:B:LEU:HG	1:68:B:LEU:H	5	0.12	0.02	0.11
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD1	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD2	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD1	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD2	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD1	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD2	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD1	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD2	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD1	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD2	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD1	5	0.12	0.03	0.11
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD2	5	0.12	0.03	0.11
(1,1623)	1:39:B:PRO:HB2	1:40:B:LEU:HA	5	0.12	0.01	0.12
(1,1623)	1:39:B:PRO:HB3	1:40:B:LEU:HA	5	0.12	0.01	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG11	5	0.12	0.01	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG12	5	0.12	0.01	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG13	5	0.12	0.01	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG21	5	0.12	0.01	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG22	5	0.12	0.01	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG23	5	0.12	0.01	0.12
(1,1727)	1:58:B:ILE:HB	1:64:B:ASP:HA	5	0.12	0.01	0.12
(1,2275)	1:24:B:VAL:HG11	1:36:B:LEU:HG	5	0.12	0.0	0.12
(1,2275)	1:24:B:VAL:HG12	1:36:B:LEU:HG	5	0.12	0.0	0.12
(1,2275)	1:24:B:VAL:HG13	1:36:B:LEU:HG	5	0.12	0.0	0.12
(1,2275)	1:24:B:VAL:HG21	1:36:B:LEU:HG	5	0.12	0.0	0.12
(1,2275)	1:24:B:VAL:HG22	1:36:B:LEU:HG	5	0.12	0.0	0.12
(1,2275)	1:24:B:VAL:HG23	1:36:B:LEU:HG	5	0.12	0.0	0.12
(1,251)	1:19:A:PRO:HG2	1:41:A:THR:HB	5	0.11	0.01	0.11
(1,251)	1:19:A:PRO:HG3	1:41:A:THR:HB	5	0.11	0.01	0.11
(1,1356)	1:102:A:ILE:HG22	1:101:A:LEU:HG	4	0.47	0.17	0.43
(1,1356)	1:102:A:ILE:HG13	1:101:A:LEU:HG	4	0.47	0.17	0.43
(1,1356)	1:102:A:ILE:HG12	1:101:A:LEU:HG	4	0.47	0.17	0.43
(1,1696)	1:58:B:ILE:HG13	1:57:B:THR:HB	4	0.29	0.07	0.27
(1,1696)	1:58:B:ILE:HG12	1:57:B:THR:HB	4	0.29	0.07	0.27
(1,312)	1:58:A:ILE:HG13	1:57:A:THR:HB	4	0.24	0.14	0.19
(1,312)	1:58:A:ILE:HG23	1:57:A:THR:HB	4	0.24	0.14	0.19
(1,66)	1:17:A:THR:HG1	1:16:A:LYS:HB3	4	0.22	0.06	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,66)	1:17:A:THR:HG1	1:16:A:LYS:HB2	4	0.22	0.06	0.22
(1,1710)	1:60:B:ILE:HG21	1:58:B:ILE:HG12	4	0.17	0.02	0.16
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB2	4	0.16	0.02	0.15
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB3	4	0.16	0.02	0.15
(1,1801)	1:37:B:VAL:HG22	1:73:B:THR:HG22	4	0.16	0.06	0.14
(1,1801)	1:37:B:VAL:HG23	1:73:B:THR:HG1	4	0.16	0.06	0.14
(1,1801)	1:37:B:VAL:HG23	1:73:B:THR:HG22	4	0.16	0.06	0.14
(1,1801)	1:37:B:VAL:HG22	1:73:B:THR:HG23	4	0.16	0.06	0.14
(1,1828)	1:34:B:THR:HG22	1:76:B:PRO:HG3	4	0.14	0.01	0.15
(1,1828)	1:34:B:THR:HG21	1:76:B:PRO:HG3	4	0.14	0.01	0.15
(1,639)	1:94:A:ILE:HG21	1:4:A:PHE:HE1	4	0.14	0.03	0.12
(1,585)	1:58:A:ILE:HB	1:90:A:PHE:HZ	4	0.12	0.02	0.12
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB2	4	0.12	0.02	0.12
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB3	4	0.12	0.02	0.12
(1,1763)	1:42:B:PRO:HA	1:66:B:ILE:HG13	4	0.12	0.01	0.12
(1,650)	1:91:A:ARG:HB2	1:95:A:ILE:HG13	4	0.12	0.01	0.12
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG2	4	0.12	0.01	0.12
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG3	4	0.12	0.01	0.12
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB2	4	0.11	0.01	0.12
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB3	4	0.11	0.01	0.12
(1,1666)	1:47:B:ASP:HB2	1:48:B:LYS:HA	4	0.11	0.0	0.11
(1,1666)	1:47:B:ASP:HB3	1:48:B:LYS:HA	4	0.11	0.0	0.11
(1,262)	1:43:A:ILE:HD11	1:43:A:ILE:HB	4	0.11	0.0	0.11
(1,262)	1:43:A:ILE:HD12	1:43:A:ILE:HB	4	0.11	0.0	0.11
(1,262)	1:43:A:ILE:HD13	1:43:A:ILE:HB	4	0.11	0.0	0.11
(1,1656)	1:46:B:LEU:HB2	1:41:B:THR:HG1	3	0.79	0.11	0.75
(1,1656)	1:46:B:LEU:HB2	1:41:B:THR:HG22	3	0.79	0.11	0.75
(1,2740)	1:102:B:ILE:HG12	1:101:B:LEU:HG	3	0.72	0.02	0.72
(1,1726)	1:57:B:THR:HG22	1:64:B:ASP:HB3	3	0.56	0.18	0.57
(1,1726)	1:57:B:THR:HG1	1:64:B:ASP:HB3	3	0.56	0.18	0.57
(1,1726)	1:57:B:THR:HG23	1:64:B:ASP:HB3	3	0.56	0.18	0.57
(1,1289)	1:94:A:ILE:HG12	1:90:A:PHE:HB3	3	0.48	0.12	0.4
(1,1289)	1:94:A:ILE:HG13	1:90:A:PHE:HB3	3	0.48	0.12	0.4
(1,1289)	1:94:A:ILE:HG12	1:90:A:PHE:HB2	3	0.48	0.12	0.4
(1,1720)	1:43:B:ILE:HG13	1:64:B:ASP:HB2	3	0.39	0.22	0.4
(1,1720)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	3	0.39	0.22	0.4
(1,1288)	1:94:A:ILE:HG12	1:90:A:PHE:HB3	3	0.38	0.12	0.3
(1,1288)	1:94:A:ILE:HG13	1:90:A:PHE:HB3	3	0.38	0.12	0.3
(1,1288)	1:94:A:ILE:HG12	1:90:A:PHE:HB2	3	0.38	0.12	0.3
(1,1376)	1:103:A:THR:HG21	1:103:A:THR:HA	3	0.32	0.09	0.28
(1,1376)	1:103:A:THR:HG23	1:103:A:THR:HA	3	0.32	0.09	0.28
(1,1376)	1:103:A:THR:HG1	1:103:A:THR:HA	3	0.32	0.09	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1285)	1:94:A:ILE:HG21	1:4:A:PHE:HD1	3	0.31	0.13	0.36
(1,1287)	1:90:A:PHE:HB3	1:94:A:ILE:HG12	3	0.31	0.12	0.23
(1,1287)	1:90:A:PHE:HB3	1:94:A:ILE:HG13	3	0.31	0.12	0.23
(1,1287)	1:90:A:PHE:HB2	1:94:A:ILE:HG12	3	0.31	0.12	0.23
(1,2921)	1:58:A:ILE:H	1:58:A:ILE:HG21	3	0.29	0.02	0.28
(1,2803)	1:60:A:ILE:H	1:58:A:ILE:HG21	3	0.28	0.13	0.33
(1,2803)	1:60:A:ILE:H	1:58:A:ILE:HG13	3	0.28	0.13	0.33
(1,3179)	1:58:B:ILE:H	1:58:B:ILE:HG21	3	0.25	0.05	0.28
(1,444)	1:34:A:THR:HG23	1:76:A:PRO:HG3	3	0.19	0.02	0.18
(1,444)	1:34:A:THR:HG22	1:76:A:PRO:HG3	3	0.19	0.02	0.18
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG11	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG12	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG13	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG21	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG22	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG23	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG11	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG12	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG13	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG21	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG22	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG23	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG11	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG12	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG13	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG21	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG22	3	0.17	0.07	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG23	3	0.17	0.07	0.15
(1,1961)	1:90:B:PHE:HE1	1:57:B:THR:HB	3	0.13	0.02	0.13
(1,1961)	1:90:B:PHE:HE2	1:57:B:THR:HB	3	0.13	0.02	0.13
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB2	3	0.12	0.01	0.13
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB3	3	0.12	0.01	0.13
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD1	3	0.12	0.0	0.12
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD2	3	0.12	0.0	0.12
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD1	3	0.12	0.0	0.12
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD2	3	0.12	0.0	0.12
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD1	3	0.12	0.0	0.12
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD2	3	0.12	0.0	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD1	3	0.12	0.0	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD2	3	0.12	0.0	0.12
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD1	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD2	3	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD1	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD2	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD1	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD2	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD1	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD2	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD1	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD2	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD1	3	0.12	0.02	0.11
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD2	3	0.12	0.02	0.11
(1,2767)	1:105:B:ILE:HD11	1:105:B:ILE:HA	3	0.12	0.01	0.11
(1,2767)	1:105:B:ILE:HD12	1:105:B:ILE:HA	3	0.12	0.01	0.11
(1,2767)	1:105:B:ILE:HD13	1:105:B:ILE:HA	3	0.12	0.01	0.11
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD11	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD12	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD13	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD11	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD12	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD13	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD11	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD12	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD13	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD11	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD12	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD13	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD11	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD12	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD13	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD11	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD12	3	0.11	0.01	0.11
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD13	3	0.11	0.01	0.11
(1,320)	1:58:A:ILE:HB	1:58:A:ILE:H	3	0.11	0.0	0.11
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB2	3	0.11	0.01	0.11
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB3	3	0.11	0.01	0.11
(1,2034)	1:91:B:ARG:HB2	1:95:B:ILE:HG13	3	0.11	0.01	0.11
(1,2673)	1:94:B:ILE:HG13	1:90:B:PHE:HB3	2	0.58	0.1	0.58
(1,2672)	1:94:B:ILE:HG13	1:90:B:PHE:HB3	2	0.48	0.1	0.48
(1,643)	1:94:A:ILE:HG21	1:24:A:VAL:HG22	2	0.44	0.19	0.44
(1,643)	1:94:A:ILE:HG21	1:24:A:VAL:HG21	2	0.44	0.19	0.44
(1,2811)	1:66:A:ILE:H	1:43:A:ILE:HG13	2	0.44	0.32	0.44
(1,2671)	1:90:B:PHE:HB3	1:94:B:ILE:HG13	2	0.42	0.11	0.42
(1,342)	1:57:A:THR:HG21	1:64:A:ASP:HB3	2	0.36	0.13	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,342)	1:57:A:THR:HG23	1:64:A:ASP:HB3	2	0.36	0.13	0.36
(1,3069)	1:66:B:ILE:H	1:43:B:ILE:HG22	2	0.34	0.24	0.34
(1,3069)	1:66:B:ILE:H	1:43:B:ILE:HG13	2	0.34	0.24	0.34
(1,3061)	1:60:B:ILE:H	1:58:B:ILE:HG13	2	0.32	0.1	0.32
(1,3061)	1:60:B:ILE:H	1:58:B:ILE:HG21	2	0.32	0.1	0.32
(1,321)	1:59:A:HIS:HB2	1:57:A:THR:HG23	2	0.31	0.19	0.31
(1,321)	1:59:A:HIS:HB2	1:57:A:THR:HG1	2	0.31	0.19	0.31
(1,2847)	1:10:A:LYS:H	1:10:A:LYS:HG2	2	0.31	0.02	0.31
(1,2847)	1:10:A:LYS:H	1:10:A:LYS:HG3	2	0.31	0.02	0.31
(1,1767)	1:56:B:PRO:HA	1:66:B:ILE:HG21	2	0.3	0.04	0.3
(1,1716)	1:61:B:ASP:HB3	1:60:B:ILE:HG13	2	0.3	0.1	0.3
(1,1724)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	2	0.3	0.12	0.3
(1,332)	1:61:A:ASP:HB3	1:60:A:ILE:HG13	2	0.26	0.02	0.26
(1,332)	1:61:A:ASP:HB2	1:60:A:ILE:HG13	2	0.26	0.02	0.26
(1,54)	1:10:A:LYS:HD2	1:14:A:SER:HB2	2	0.23	0.02	0.23
(1,54)	1:10:A:LYS:HD2	1:14:A:SER:HB3	2	0.23	0.02	0.23
(1,54)	1:10:A:LYS:HD3	1:14:A:SER:HB2	2	0.23	0.02	0.23
(1,54)	1:10:A:LYS:HD3	1:14:A:SER:HB3	2	0.23	0.02	0.23
(1,992)	1:58:A:ILE:HG13	1:56:A:PRO:HB2	2	0.21	0.04	0.21
(1,992)	1:58:A:ILE:HG21	1:56:A:PRO:HB2	2	0.21	0.04	0.21
(1,306)	1:56:A:PRO:HB2	1:58:A:ILE:HG13	2	0.19	0.04	0.19
(1,306)	1:56:A:PRO:HB2	1:58:A:ILE:HG21	2	0.19	0.04	0.19
(1,997)	1:58:A:ILE:HA	1:58:A:ILE:HG13	2	0.18	0.04	0.18
(1,1570)	1:34:B:THR:HA	1:34:B:THR:HG22	2	0.18	0.03	0.18
(1,2348)	1:42:B:PRO:HB2	1:45:B:LEU:HG	2	0.15	0.03	0.15
(1,2348)	1:42:B:PRO:HB3	1:45:B:LEU:HG	2	0.15	0.03	0.15
(1,1795)	1:69:B:THR:HG1	1:69:B:THR:HA	2	0.15	0.0	0.15
(1,471)	1:79:A:ILE:HD11	1:75:A:VAL:HA	2	0.14	0.02	0.14
(1,471)	1:79:A:ILE:HD12	1:75:A:VAL:HA	2	0.14	0.02	0.14
(1,471)	1:79:A:ILE:HD13	1:75:A:VAL:HA	2	0.14	0.02	0.14
(1,1073)	1:56:A:PRO:HD2	1:67:A:MET:HG2	2	0.14	0.02	0.14
(1,1073)	1:56:A:PRO:HD2	1:67:A:MET:HG3	2	0.14	0.02	0.14
(1,1073)	1:56:A:PRO:HD3	1:67:A:MET:HG2	2	0.14	0.02	0.14
(1,1073)	1:56:A:PRO:HD3	1:67:A:MET:HG3	2	0.14	0.02	0.14
(1,237)	1:40:A:LEU:HD11	1:20:A:TYR:HE1	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD11	1:20:A:TYR:HE2	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD12	1:20:A:TYR:HE1	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD12	1:20:A:TYR:HE2	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD13	1:20:A:TYR:HE1	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD13	1:20:A:TYR:HE2	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD21	1:20:A:TYR:HE1	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD21	1:20:A:TYR:HE2	2	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,237)	1:40:A:LEU:HD22	1:20:A:TYR:HE1	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD22	1:20:A:TYR:HE2	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD23	1:20:A:TYR:HE1	2	0.13	0.01	0.13
(1,237)	1:40:A:LEU:HD23	1:20:A:TYR:HE2	2	0.13	0.01	0.13
(1,248)	1:40:A:LEU:HG	1:40:A:LEU:HB2	2	0.12	0.02	0.12
(1,248)	1:40:A:LEU:HG	1:40:A:LEU:HB3	2	0.12	0.02	0.12
(1,379)	1:42:A:PRO:HA	1:66:A:ILE:HG13	2	0.12	0.02	0.12
(1,2792)	1:36:A:LEU:H	1:24:A:VAL:H	2	0.12	0.02	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG11	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG12	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG13	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG21	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG22	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG23	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG11	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG12	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG13	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG21	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG22	2	0.12	0.0	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG23	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG11	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG12	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG13	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG21	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG22	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG23	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG11	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG12	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG13	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG21	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG22	2	0.12	0.0	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG23	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG11	1:8:B:LYS:HB2	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG11	1:8:B:LYS:HB3	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG12	1:8:B:LYS:HB2	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG12	1:8:B:LYS:HB3	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG13	1:8:B:LYS:HB2	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG13	1:8:B:LYS:HB3	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG21	1:8:B:LYS:HB2	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG21	1:8:B:LYS:HB3	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG22	1:8:B:LYS:HB2	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG22	1:8:B:LYS:HB3	2	0.12	0.0	0.12

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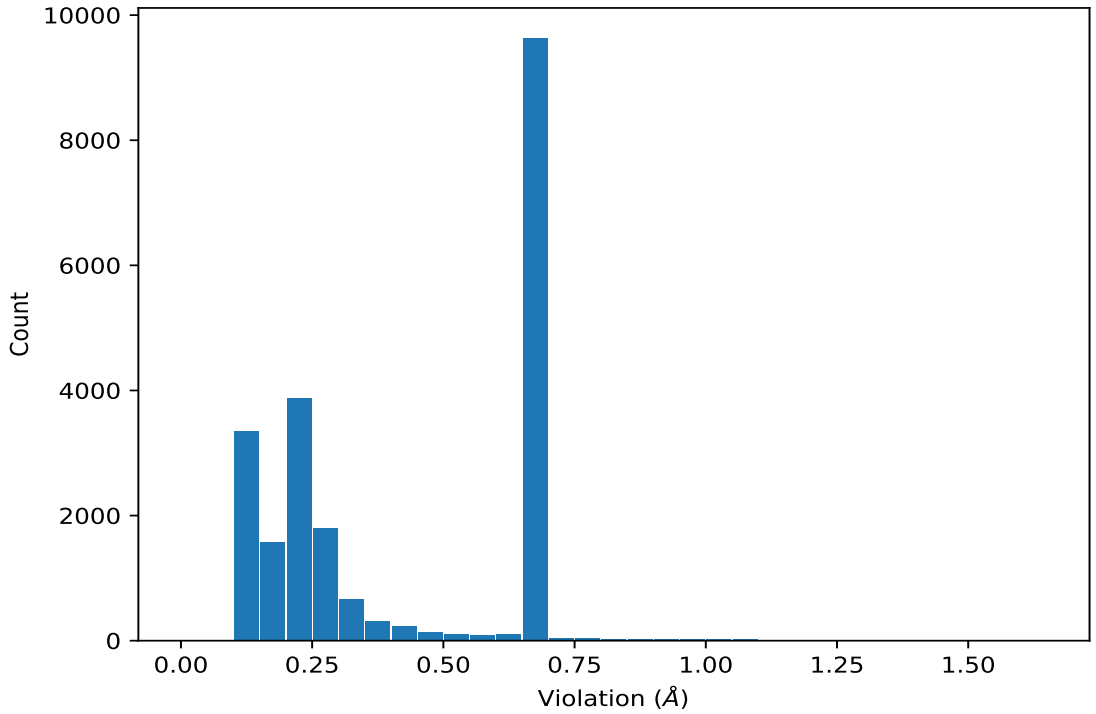
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2596)	1:84:B:VAL:HG23	1:8:B:LYS:HB2	2	0.12	0.0	0.12
(1,2596)	1:84:B:VAL:HG23	1:8:B:LYS:HB3	2	0.12	0.0	0.12
(1,2876)	1:20:A:TYR:H	1:19:A:PRO:HG2	2	0.12	0.0	0.12
(1,2876)	1:20:A:TYR:H	1:19:A:PRO:HG3	2	0.12	0.0	0.12
(1,724)	1:99:A:ASP:HA	1:102:A:ILE:H	2	0.11	0.0	0.11
(1,1646)	1:43:B:ILE:HD11	1:43:B:ILE:HB	2	0.11	0.01	0.11
(1,1646)	1:43:B:ILE:HD12	1:43:B:ILE:HB	2	0.11	0.01	0.11
(1,1646)	1:43:B:ILE:HD13	1:43:B:ILE:HB	2	0.11	0.01	0.11
(1,1776)	1:67:B:MET:HG2	1:21:B:PHE:HA	2	0.11	0.01	0.11
(1,1776)	1:67:B:MET:HG3	1:21:B:PHE:HA	2	0.11	0.01	0.11
(1,2845)	1:9:A:ASN:H	1:8:A:LYS:HA	2	0.11	0.0	0.11
(1,2906)	1:40:A:LEU:H	1:40:A:LEU:HB2	2	0.11	0.0	0.11
(1,2906)	1:40:A:LEU:H	1:40:A:LEU:HB3	2	0.11	0.0	0.11
(1,405)	1:40:A:LEU:HG	1:68:A:LEU:H	2	0.11	0.0	0.11
(1,626)	1:91:A:ARG:HG2	1:92:A:ASN:HA	2	0.11	0.0	0.11
(1,626)	1:91:A:ARG:HG3	1:92:A:ASN:HA	2	0.11	0.0	0.11
(1,1854)	1:79:B:ILE:HD11	1:21:B:PHE:HD1	2	0.11	0.0	0.11
(1,1854)	1:79:B:ILE:HD11	1:21:B:PHE:HD2	2	0.11	0.0	0.11
(1,1854)	1:79:B:ILE:HD12	1:21:B:PHE:HD1	2	0.11	0.0	0.11
(1,1854)	1:79:B:ILE:HD12	1:21:B:PHE:HD2	2	0.11	0.0	0.11
(1,1854)	1:79:B:ILE:HD13	1:21:B:PHE:HD1	2	0.11	0.0	0.11
(1,1854)	1:79:B:ILE:HD13	1:21:B:PHE:HD2	2	0.11	0.0	0.11
(1,2023)	1:94:B:ILE:HG13	1:4:B:PHE:HE1	2	0.11	0.0	0.11
(1,2062)	1:96:B:ALA:HA	1:99:B:ASP:HA	2	0.11	0.0	0.11
(1,2760)	1:103:B:THR:HG21	1:103:B:THR:HA	2	0.1	0.0	0.1

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	20	1.62
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	19	1.57
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	19	1.56
(1,2031)	1:93:B:GLU:HG3	1:94:B:ILE:HG13	15	1.49
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	11	1.47
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	19	1.47
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	7	1.46
(1,2031)	1:93:B:GLU:HG3	1:94:B:ILE:HG13	9	1.39
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	16	1.39
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	13	1.35
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	14	1.35
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	8	1.34
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	11	1.33
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	6	1.33
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	8	1.31
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	5	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	20	1.28
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	12	1.27
(1,2326)	1:17:B:THR:HG21	1:41:B:THR:HG1	1	1.24
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	9	1.24
(1,2465)	1:68:B:LEU:HD23	1:66:B:ILE:HG12	16	1.23
(1,2114)	1:103:B:THR:HG22	1:99:B:ASP:HB3	13	1.23
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	17	1.23
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	4	1.21
(1,1928)	1:85:B:ASN:HB2	1:60:B:ILE:HG23	4	1.2
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	1	1.2
(1,647)	1:93:A:GLU:HG3	1:94:A:ILE:HG13	15	1.19
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD13	20	1.19
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	6	1.18
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	17	1.18
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	16	1.17
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	17	1.17
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	7	1.16
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	3	1.15
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	3	1.15
(1,1711)	1:60:B:ILE:HG22	1:58:B:ILE:HD11	7	1.14
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	6	1.14
(1,2031)	1:93:B:GLU:HG3	1:94:B:ILE:HG13	14	1.13
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	18	1.13
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	18	1.13
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD11	13	1.12
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	9	1.12
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	5	1.12
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	17	1.11
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG12	11	1.11
(1,942)	1:17:A:THR:HG21	1:41:A:THR:HG1	3	1.11
(1,327)	1:60:A:ILE:HG22	1:58:A:ILE:HD11	17	1.11
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	12	1.1
(1,1711)	1:60:B:ILE:HG22	1:58:B:ILE:HD11	14	1.1
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB2	12	1.1
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	14	1.09
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	8	1.09
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	11	1.09
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD12	14	1.09
(1,1374)	1:103:A:THR:HG23	1:102:A:ILE:HG23	20	1.08
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	11	1.08
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	18	1.07
(1,2114)	1:103:B:THR:HG22	1:99:B:ASP:HB3	15	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	2	1.07
(1,2326)	1:17:B:THR:HG21	1:41:B:THR:HG1	10	1.06
(1,2114)	1:103:B:THR:HG23	1:99:B:ASP:HB2	2	1.06
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD13	16	1.06
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	10	1.06
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	20	1.06
(1,730)	1:103:A:THR:HG21	1:99:A:ASP:HB2	3	1.06
(1,2465)	1:68:B:LEU:HD13	1:66:B:ILE:HG12	11	1.05
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	7	1.05
(1,2465)	1:68:B:LEU:HD13	1:66:B:ILE:HG12	13	1.03
(1,2326)	1:17:B:THR:HG21	1:41:B:THR:HG1	2	1.03
(1,2114)	1:103:B:THR:HG22	1:99:B:ASP:HB2	17	1.03
(1,1081)	1:68:A:LEU:HD21	1:66:A:ILE:HG12	5	1.03
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	18	1.03
(1,2465)	1:68:B:LEU:HD12	1:66:B:ILE:HG12	19	1.02
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	5	1.02
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB2	18	1.02
(1,1081)	1:68:A:LEU:HD12	1:66:A:ILE:HG12	13	1.02
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG12	4	1.02
(1,2465)	1:68:B:LEU:HD12	1:66:B:ILE:HG12	14	1.01
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	17	1.01
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	2	1.01
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG21	3	1.01
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	6	1.0
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG13	2	1.0
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	5	0.99
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	12	0.99
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD13	4	0.99
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	12	0.99
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG12	13	0.99
(1,2413)	1:43:B:ILE:HG22	1:64:B:ASP:HB2	2	0.98
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	11	0.98
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	20	0.98
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	19	0.98
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	1	0.98
(1,942)	1:17:A:THR:HG21	1:41:A:THR:HG1	16	0.98
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD13	18	0.98
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	9	0.97
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	16	0.96
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG23	20	0.96
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	4	0.95
(1,2326)	1:17:B:THR:HG23	1:41:B:THR:HG1	15	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1656)	1:46:B:LEU:HB2	1:41:B:THR:HG1	17	0.95
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	16	0.95
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG13	7	0.95
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG21	8	0.95
(1,2465)	1:68:B:LEU:HD12	1:66:B:ILE:HG12	5	0.94
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	9	0.94
(1,1711)	1:60:B:ILE:HG22	1:58:B:ILE:HD12	18	0.94
(1,1081)	1:68:A:LEU:HD13	1:66:A:ILE:HG12	4	0.94
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	10	0.94
(1,942)	1:17:A:THR:HG21	1:41:A:THR:HG1	12	0.94
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	3	0.93
(1,726)	1:101:A:LEU:HB2	1:102:A:ILE:HG21	16	0.93
(1,2326)	1:17:B:THR:HG1	1:41:B:THR:HG1	13	0.92
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	19	0.92
(1,1374)	1:103:A:THR:HG22	1:102:A:ILE:HG13	19	0.92
(1,942)	1:17:A:THR:HG21	1:41:A:THR:HG1	5	0.92
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	9	0.92
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD13	5	0.92
(1,2758)	1:103:B:THR:HG22	1:102:B:ILE:HG12	11	0.91
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	20	0.91
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG12	18	0.91
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD13	3	0.91
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG23	14	0.91
(1,327)	1:60:A:ILE:HG22	1:58:A:ILE:HD12	4	0.91
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	17	0.9
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	20	0.9
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD12	17	0.9
(1,1081)	1:68:A:LEU:HD13	1:66:A:ILE:HG12	15	0.9
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	7	0.9
(1,726)	1:101:A:LEU:HB2	1:102:A:ILE:HG21	6	0.9
(1,302)	1:57:A:THR:HG23	1:43:A:ILE:HB	19	0.9
(1,2465)	1:68:B:LEU:HD13	1:66:B:ILE:HG12	4	0.89
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	9	0.89
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG12	3	0.89
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	20	0.89
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	20	0.88
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	6	0.88
(1,2110)	1:101:B:LEU:HB2	1:102:B:ILE:HG21	10	0.88
(1,2110)	1:101:B:LEU:HB2	1:102:B:ILE:HG21	11	0.88
(1,1081)	1:68:A:LEU:HD13	1:66:A:ILE:HG12	10	0.88
(1,942)	1:17:A:THR:HG23	1:41:A:THR:HG1	15	0.88
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG1	6	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG23	16	0.88
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG22	16	0.87
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	14	0.87
(1,302)	1:57:A:THR:HG23	1:43:A:ILE:HB	15	0.87
(1,1971)	1:60:B:ILE:HG21	1:90:B:PHE:HZ	2	0.86
(1,942)	1:17:A:THR:HG22	1:41:A:THR:HG1	13	0.86
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD13	20	0.86
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD11	3	0.86
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	8	0.85
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	19	0.85
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD13	11	0.85
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	8	0.85
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	10	0.85
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	2	0.84
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	10	0.84
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	8	0.84
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	14	0.84
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	16	0.84
(1,2326)	1:17:B:THR:HG22	1:41:B:THR:HG1	8	0.83
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG22	20	0.83
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG22	9	0.83
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	8	0.83
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	18	0.83
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG21	9	0.83
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	1	0.83
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	17	0.82
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG21	18	0.82
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	6	0.82
(1,2465)	1:68:B:LEU:HD13	1:66:B:ILE:HG12	18	0.81
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	9	0.81
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	11	0.81
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD12	8	0.81
(1,2758)	1:103:B:THR:HG22	1:102:B:ILE:HG12	10	0.8
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	16	0.79
(1,1081)	1:68:A:LEU:HD13	1:66:A:ILE:HG12	1	0.79
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	8	0.79
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG13	6	0.79
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG23	9	0.79
(1,730)	1:103:A:THR:HG21	1:99:A:ASP:HB3	16	0.79
(1,587)	1:60:A:ILE:HG21	1:90:A:PHE:HZ	1	0.79
(1,361)	1:43:A:ILE:HG21	1:65:A:PHE:HB3	6	0.79
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD13	9	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1726)	1:57:B:THR:HG22	1:64:B:ASP:HB3	17	0.78
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD13	20	0.78
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG21	1	0.78
(1,2697)	1:69:B:THR:HG22	1:98:B:ILE:HA	9	0.77
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	1	0.77
(1,1374)	1:103:A:THR:HG23	1:102:A:ILE:HG12	6	0.77
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG22	13	0.77
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG1	20	0.77
(1,2811)	1:66:A:ILE:H	1:43:A:ILE:HG13	6	0.76
(1,2372)	1:43:B:ILE:HG21	1:57:B:THR:HG23	20	0.76
(1,2085)	1:69:B:THR:HG23	1:101:B:LEU:HB3	7	0.76
(1,1971)	1:60:B:ILE:HG21	1:90:B:PHE:HZ	10	0.76
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	12	0.76
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	1	0.76
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	20	0.76
(1,421)	1:71:A:GLN:HB2	1:73:A:THR:HG23	2	0.76
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	20	0.76
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG21	5	0.76
(1,2740)	1:102:B:ILE:HG12	1:101:B:LEU:HG	6	0.75
(1,2465)	1:68:B:LEU:HD21	1:66:B:ILE:HG12	17	0.75
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG21	1	0.75
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	6	0.75
(1,1656)	1:46:B:LEU:HB2	1:41:B:THR:HG22	15	0.75
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	7	0.75
(1,341)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	11	0.75
(1,2465)	1:68:B:LEU:HD13	1:66:B:ILE:HG12	7	0.74
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG22	8	0.74
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	3	0.74
(1,1711)	1:60:B:ILE:HG13	1:58:B:ILE:HD11	15	0.74
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	7	0.74
(1,730)	1:103:A:THR:HG21	1:99:A:ASP:HB3	7	0.74
(1,587)	1:60:A:ILE:HG21	1:90:A:PHE:HZ	12	0.74
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	11	0.73
(1,2697)	1:69:B:THR:HG22	1:98:B:ILE:HA	19	0.73
(1,2465)	1:68:B:LEU:HD12	1:66:B:ILE:HG12	3	0.73
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	5	0.73
(1,1313)	1:69:A:THR:HG21	1:98:A:ILE:HA	8	0.73
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	4	0.73
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	6	0.73
(1,2740)	1:102:B:ILE:HG12	1:101:B:LEU:HG	13	0.72
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG13	11	0.72
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	12	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:60:A:ILE:HG21	1:90:A:PHE:HZ	6	0.72
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	3	0.72
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	14	0.72
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD13	10	0.72
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	6	0.72
(1,2465)	1:68:B:LEU:HD11	1:66:B:ILE:HG12	15	0.71
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB2	1	0.71
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG23	15	0.71
(1,1971)	1:60:B:ILE:HG21	1:90:B:PHE:HZ	6	0.71
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG21	14	0.71
(1,1356)	1:102:A:ILE:HG12	1:101:A:LEU:HG	15	0.71
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	20	0.71
(1,587)	1:60:A:ILE:HG21	1:90:A:PHE:HZ	11	0.71
(1,341)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	7	0.71
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG22	7	0.71
(1,2740)	1:102:B:ILE:HG12	1:101:B:LEU:HG	14	0.7
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	7	0.7
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG12	16	0.7
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	1	0.7
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	19	0.7
(1,341)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	18	0.7
(1,338)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	11	0.7
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	13	0.69
(1,2697)	1:69:B:THR:HG22	1:98:B:ILE:HA	5	0.69
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	16	0.69
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	18	0.69
(1,2673)	1:94:B:ILE:HG13	1:90:B:PHE:HB3	6	0.69
(1,2465)	1:68:B:LEU:HD12	1:66:B:ILE:HG12	12	0.69
(1,2085)	1:69:B:THR:HG23	1:101:B:LEU:HB3	18	0.69
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	20	0.69
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	2	0.69
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD12	12	0.69
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	9	0.69
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG22	11	0.69
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	8	0.69
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD13	2	0.69
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG23	19	0.69
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	7	0.68
(1,2697)	1:69:B:THR:HG21	1:98:B:ILE:HA	10	0.68
(1,2697)	1:69:B:THR:HG21	1:98:B:ILE:HA	20	0.68
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	16	0.68
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG13	10	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG21	2	0.68
(1,1656)	1:46:B:LEU:HB2	1:41:B:THR:HG1	10	0.68
(1,1374)	1:103:A:THR:HG21	1:102:A:ILE:HG13	15	0.68
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	2	0.68
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	7	0.67
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	13	0.67
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	15	0.67
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	5	0.67
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	7	0.67
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG23	14	0.67
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG21	5	0.67
(1,575)	1:89:A:THR:HG23	1:87:A:LEU:HB2	9	0.67
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	6	0.67
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	14	0.67
(1,338)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	7	0.67
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG23	7	0.67
(1,2697)	1:69:B:THR:HG21	1:98:B:ILE:HA	13	0.66
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	3	0.66
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB2	5	0.66
(1,2114)	1:103:B:THR:HG21	1:99:B:ASP:HB3	7	0.66
(1,1725)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	5	0.66
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	19	0.66
(1,1289)	1:94:A:ILE:HG12	1:90:A:PHE:HB2	7	0.66
(1,1081)	1:68:A:LEU:HD13	1:66:A:ILE:HG12	2	0.66
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	14	0.66
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB3	11	0.66
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	13	0.66
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	17	0.66
(1,338)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	18	0.66
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	17	0.66
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG21	14	0.66
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	1	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	1	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	1	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	1	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	1	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	1	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	1	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	1	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	1	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	1	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	1	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	1	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	1	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	1	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	1	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	1	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	1	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	1	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	1	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	1	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	1	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	1	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	1	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	1	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	1	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	1	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	1	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	1	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	1	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	2	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	2	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	2	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	2	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	2	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	2	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	2	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	2	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	2	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	2	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	2	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	2	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	2	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	2	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	2	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	2	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	2	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	2	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	2	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	2	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	2	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	2	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	2	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	2	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	2	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	2	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	2	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	2	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	2	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	3	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	3	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	3	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	3	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	3	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	3	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	3	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	3	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	3	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	3	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	3	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	3	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	3	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	3	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	3	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	3	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	3	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	3	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	3	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	3	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	3	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	3	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	3	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	3	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	3	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	3	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	3	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	3	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	3	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	3	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	4	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	4	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	4	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	4	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	4	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	4	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	4	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	4	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	4	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	4	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	4	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	4	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	4	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	4	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	4	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	4	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	4	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	4	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	4	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	4	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	4	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	4	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	4	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	4	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	4	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	4	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	4	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	4	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	4	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	5	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	5	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	5	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	5	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	5	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	5	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	5	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	5	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	5	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	5	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	5	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	5	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	5	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	5	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	5	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	5	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	5	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	5	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	5	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	5	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	5	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	5	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	5	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	5	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	5	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	5	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	5	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	5	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	5	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	6	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	6	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	6	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	6	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	6	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	6	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	6	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	6	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	6	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	6	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	6	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	6	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	6	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	6	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	6	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	6	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	6	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	6	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	6	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	6	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	6	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	6	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	6	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	6	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	6	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	6	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	6	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	6	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	6	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	7	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	7	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	7	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	7	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	7	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	7	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	7	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	7	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	7	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	7	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	7	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	7	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	7	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	7	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	7	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	7	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	7	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	7	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	7	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	7	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	7	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	7	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	7	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	7	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	7	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	7	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	7	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	7	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	7	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	7	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	8	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	8	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	8	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	8	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	8	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	8	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	8	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	8	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	8	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	8	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	8	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	8	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	8	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	8	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	8	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	8	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	8	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	8	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	8	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	8	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	8	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	8	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	8	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	8	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	8	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	8	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	8	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	8	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	8	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	9	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	9	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	9	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	9	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	9	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	9	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	9	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	9	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	9	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	9	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	9	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	9	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	9	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	9	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	9	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	9	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	9	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	9	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	9	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	9	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	9	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	9	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	9	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	9	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	9	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	9	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	9	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	9	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	9	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	10	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	10	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	10	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	10	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	10	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	10	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	10	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	10	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	10	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	10	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	10	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	10	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	10	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	10	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	10	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	10	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	10	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	10	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	10	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	10	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	10	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	10	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	10	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	10	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	10	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	10	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	10	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	10	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	10	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	10	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	11	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	11	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	11	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	11	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	11	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	11	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	11	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	11	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	11	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	11	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	11	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	11	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	11	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	11	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	11	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	11	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	11	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	11	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	11	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	11	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	11	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	11	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	11	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	11	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	11	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	11	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	11	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	11	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	11	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	12	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	12	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	12	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	12	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	12	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	12	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	12	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	12	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	12	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	12	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	12	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	12	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	12	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	12	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	12	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	12	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	12	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	12	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	12	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	12	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	12	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	12	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	12	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	12	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	12	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	12	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	12	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	12	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	12	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	13	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	13	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	13	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	13	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	13	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	13	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	13	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	13	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	13	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	13	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	13	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	13	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	13	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	13	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	13	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	13	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	13	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	13	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	13	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	13	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	13	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	13	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	13	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	13	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	13	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	13	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	13	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	13	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	13	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	14	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	14	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	14	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	14	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	14	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	14	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	14	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	14	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	14	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	14	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	14	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	14	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	14	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	14	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	14	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	14	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	14	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	14	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	14	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	14	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	14	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	14	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	14	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	14	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	14	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	14	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	14	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	14	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	14	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	14	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	15	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	15	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	15	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	15	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	15	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	15	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	15	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	15	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	15	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	15	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	15	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	15	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	15	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	15	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	15	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	15	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	15	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	15	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	15	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	15	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	15	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	15	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	15	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	15	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	15	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	15	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	15	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	15	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	15	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	16	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	16	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	16	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	16	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	16	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	16	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	16	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	16	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	16	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	16	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	16	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	16	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	16	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	16	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	16	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	16	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	16	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	16	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	16	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	16	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	16	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	16	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	16	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	16	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	16	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	16	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	16	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	16	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	16	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	17	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	17	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	17	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	17	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	17	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	17	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	17	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	17	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	17	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	17	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	17	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	17	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	17	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	17	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	17	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	17	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	17	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	17	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	17	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	17	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	17	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	17	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	17	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	17	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	17	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	17	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	17	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	17	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	17	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	17	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	18	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	18	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	18	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	18	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	18	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	18	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	18	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	18	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	18	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	18	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	18	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	18	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	18	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	18	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	18	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	18	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	18	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	18	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	18	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	18	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	18	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	18	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	18	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	18	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	18	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	18	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	18	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	18	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	18	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	20	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	20	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	20	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	20	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	20	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	20	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	20	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	20	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	20	0.65
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	20	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	20	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	20	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	20	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	20	0.65
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	20	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	20	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	20	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	20	0.65
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	20	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	20	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	20	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	20	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	20	0.65
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	20	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	20	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	20	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	20	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	20	0.65
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	20	0.65
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	3	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	1	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	1	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	1	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	1	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	1	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	1	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	1	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	1	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	1	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	1	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	1	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	1	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	1	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	1	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	1	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	1	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	1	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	1	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	1	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	1	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	1	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	1	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	1	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	1	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	1	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	1	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	1	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	1	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	1	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	2	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	2	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	2	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	2	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	2	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	2	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	2	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	2	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	2	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	2	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	2	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	2	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	2	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	2	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	2	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	2	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	2	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	2	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	2	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	2	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	2	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	2	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	2	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	2	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	2	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	2	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	2	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	2	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	2	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	2	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	3	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	3	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	3	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	3	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	3	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	3	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	3	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	3	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	3	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	3	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	3	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	3	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	3	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	3	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	3	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	3	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	3	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	3	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	3	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	3	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	3	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	3	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	3	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	3	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	3	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	3	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	3	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	3	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	3	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	4	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	4	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	4	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	4	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	4	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	4	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	4	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	4	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	4	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	4	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	4	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	4	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	4	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	4	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	4	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	4	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	4	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	4	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	4	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	4	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	4	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	4	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	4	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	4	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	4	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	4	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	4	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	4	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	4	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	5	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	5	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	5	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	5	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	5	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	5	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	5	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	5	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	5	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	5	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	5	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	5	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	5	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	5	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	5	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	5	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	5	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	5	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	5	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	5	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	5	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	5	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	5	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	5	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	5	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	5	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	5	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	5	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	5	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	5	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	6	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	6	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	6	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	6	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	6	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	6	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	6	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	6	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	6	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	6	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	6	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	6	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	6	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	6	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	6	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	6	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	6	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	6	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	6	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	6	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	6	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	6	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	6	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	6	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	6	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	6	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	6	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	6	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	6	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	7	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	7	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	7	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	7	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	7	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	7	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	7	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	7	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	7	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	7	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	7	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	7	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	7	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	7	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	7	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	7	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	7	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	7	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	7	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	7	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	7	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	7	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	7	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	7	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	7	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	7	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	7	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	7	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	7	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	8	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	8	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	8	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	8	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	8	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	8	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	8	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	8	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	8	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	8	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	8	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	8	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	8	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	8	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	8	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	8	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	8	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	8	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	8	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	8	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	8	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	8	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	8	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	8	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	8	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	8	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	8	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	8	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	8	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	9	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	9	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	9	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	9	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	9	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	9	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	9	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	9	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	9	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	9	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	9	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	9	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	9	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	9	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	9	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	9	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	9	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	9	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	9	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	9	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	9	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	9	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	9	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	9	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	9	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	9	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	9	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	9	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	9	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	9	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	10	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	10	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	10	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	10	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	10	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	10	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	10	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	10	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	10	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	10	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	10	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	10	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	10	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	10	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	10	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	10	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	10	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	10	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	10	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	10	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	10	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	10	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	10	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	10	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	10	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	10	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	10	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	10	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	10	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	11	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	11	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	11	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	11	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	11	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	11	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	11	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	11	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	11	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	11	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	11	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	11	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	11	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	11	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	11	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	11	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	11	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	11	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	11	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	11	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	11	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	11	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	11	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	11	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	11	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	11	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	11	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	11	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	11	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	12	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	12	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	12	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	12	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	12	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	12	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	12	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	12	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	12	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	12	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	12	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	12	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	12	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	12	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	12	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	12	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	12	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	12	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	12	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	12	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	12	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	12	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	12	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	12	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	12	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	12	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	12	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	12	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	12	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	12	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	13	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	13	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	13	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	13	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	13	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	13	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	13	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	13	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	13	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	13	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	13	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	13	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	13	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	13	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	13	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	13	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	13	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	13	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	13	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	13	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	13	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	13	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	13	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	13	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	13	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	13	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	13	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	13	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	13	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	14	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	14	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	14	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	14	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	14	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	14	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	14	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	14	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	14	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	14	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	14	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	14	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	14	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	14	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	14	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	14	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	14	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	14	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	14	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	14	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	14	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	14	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	14	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	14	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	14	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	14	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	14	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	14	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	14	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	15	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	15	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	15	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	15	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	15	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	15	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	15	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	15	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	15	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	15	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	15	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	15	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	15	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	15	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	15	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	15	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	15	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	15	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	15	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	15	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	15	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	15	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	15	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	15	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	15	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	15	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	15	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	15	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	15	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	16	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	16	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	16	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	16	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	16	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	16	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	16	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	16	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	16	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	16	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	16	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	16	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	16	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	16	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	16	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	16	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	16	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	16	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	16	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	16	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	16	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	16	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	16	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	16	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	16	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	16	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	16	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	16	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	16	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	16	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	17	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	17	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	17	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	17	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	17	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	17	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	17	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	17	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	17	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	17	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	17	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	17	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	17	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	17	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	17	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	17	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	17	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	17	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	17	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	17	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	17	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	17	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	17	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	17	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	17	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	17	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	17	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	17	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	17	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	18	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	18	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	18	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	18	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	18	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	18	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	18	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	18	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	18	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	18	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	18	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	18	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	18	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	18	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	18	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	18	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	18	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	18	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	18	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	18	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	18	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	18	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	18	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	18	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	18	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	18	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	18	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	18	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	18	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	19	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	19	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	19	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	19	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	19	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	19	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	19	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	19	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	19	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	19	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	19	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	19	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	19	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	19	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	19	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	19	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	19	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	19	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	19	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	19	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	19	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	19	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	19	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	19	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	19	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	19	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	19	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	19	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	19	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	19	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	20	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	20	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	20	0.65
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	20	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	20	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	20	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	20	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	20	0.65
(1,2607)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	20	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	20	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	20	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	20	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	20	0.65
(1,2607)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	20	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	20	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	20	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	20	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	20	0.65
(1,2607)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	20	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	20	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	20	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	20	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	20	0.65
(1,2607)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	20	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	20	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	20	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	20	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	20	0.65
(1,2607)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	20	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	1	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	1	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	1	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	1	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	1	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	1	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	1	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	1	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	1	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	1	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	1	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	1	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	1	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	1	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	1	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	1	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	1	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	1	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	1	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	1	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	1	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	1	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	1	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	1	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	1	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	1	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	1	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	1	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	1	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	2	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	2	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	2	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	2	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	2	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	2	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	2	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	2	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	2	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	2	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	2	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	2	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	2	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	2	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	2	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	2	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	2	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	2	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	2	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	2	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	2	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	2	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	2	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	2	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	2	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	2	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	2	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	2	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	2	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	3	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	3	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	3	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	3	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	3	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	3	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	3	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	3	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	3	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	3	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	3	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	3	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	3	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	3	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	3	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	3	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	3	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	3	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	3	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	3	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	3	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	3	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	3	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	3	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	3	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	3	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	3	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	3	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	3	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	3	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	4	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	4	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	4	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	4	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	4	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	4	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	4	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	4	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	4	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	4	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	4	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	4	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	4	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	4	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	4	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	4	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	4	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	4	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	4	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	4	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	4	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	4	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	4	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	4	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	4	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	4	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	4	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	4	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	4	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	5	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	5	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	5	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	5	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	5	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	5	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	5	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	5	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	5	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	5	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	5	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	5	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	5	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	5	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	5	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	5	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	5	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	5	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	5	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	5	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	5	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	5	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	5	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	5	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	5	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	5	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	5	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	5	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	5	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	6	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	6	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	6	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	6	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	6	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	6	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	6	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	6	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	6	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	6	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	6	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	6	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	6	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	6	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	6	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	6	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	6	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	6	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	6	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	6	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	6	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	6	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	6	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	6	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	6	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	6	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	6	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	6	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	6	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	6	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	7	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	7	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	7	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	7	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	7	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	7	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	7	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	7	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	7	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	7	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	7	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	7	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	7	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	7	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	7	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	7	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	7	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	7	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	7	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	7	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	7	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	7	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	7	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	7	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	7	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	7	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	7	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	7	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	7	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	8	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	8	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	8	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	8	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	8	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	8	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	8	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	8	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	8	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	8	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	8	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	8	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	8	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	8	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	8	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	8	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	8	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	8	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	8	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	8	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	8	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	8	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	8	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	8	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	8	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	8	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	8	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	8	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	8	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	9	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	9	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	9	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	9	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	9	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	9	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	9	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	9	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	9	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	9	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	9	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	9	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	9	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	9	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	9	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	9	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	9	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	9	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	9	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	9	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	9	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	9	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	9	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	9	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	9	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	9	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	9	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	9	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	9	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	10	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	10	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	10	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	10	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	10	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	10	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	10	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	10	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	10	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	10	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	10	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	10	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	10	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	10	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	10	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	10	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	10	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	10	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	10	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	10	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	10	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	10	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	10	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	10	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	10	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	10	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	10	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	10	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	10	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	10	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	11	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	11	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	11	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	11	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	11	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	11	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	11	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	11	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	11	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	11	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	11	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	11	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	11	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	11	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	11	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	11	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	11	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	11	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	11	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	11	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	11	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	11	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	11	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	11	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	11	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	11	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	11	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	11	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	11	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	12	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	12	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	12	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	12	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	12	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	12	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	12	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	12	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	12	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	12	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	12	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	12	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	12	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	12	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	12	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	12	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	12	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	12	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	12	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	12	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	12	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	12	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	12	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	12	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	12	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	12	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	12	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	12	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	12	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	13	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	13	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	13	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	13	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	13	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	13	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	13	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	13	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	13	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	13	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	13	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	13	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	13	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	13	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	13	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	13	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	13	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	13	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	13	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	13	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	13	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	13	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	13	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	13	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	13	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	13	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	13	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	13	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	13	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	13	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	14	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	14	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	14	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	14	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	14	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	14	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	14	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	14	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	14	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	14	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	14	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	14	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	14	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	14	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	14	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	14	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	14	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	14	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	14	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	14	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	14	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	14	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	14	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	14	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	14	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	14	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	14	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	14	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	14	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	15	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	15	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	15	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	15	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	15	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	15	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	15	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	15	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	15	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	15	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	15	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	15	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	15	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	15	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	15	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	15	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	15	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	15	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	15	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	15	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	15	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	15	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	15	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	15	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	15	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	15	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	15	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	15	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	15	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	16	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	16	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	16	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	16	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	16	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	16	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	16	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	16	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	16	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	16	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	16	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	16	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	16	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	16	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	16	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	16	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	16	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	16	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	16	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	16	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	16	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	16	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	16	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	16	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	16	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	16	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	16	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	16	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	16	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	17	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	17	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	17	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	17	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	17	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	17	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	17	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	17	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	17	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	17	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	17	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	17	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	17	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	17	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	17	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	17	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	17	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	17	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	17	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	17	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	17	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	17	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	17	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	17	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	17	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	17	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	17	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	17	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	17	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	17	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	18	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	18	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	18	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	18	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	18	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	18	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	18	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	18	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	18	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	18	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	18	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	18	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	18	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	18	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	18	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	18	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	18	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	18	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	18	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	18	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	18	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	18	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	18	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	18	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	18	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	18	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	18	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	18	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	18	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	19	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	19	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	19	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	19	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	19	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	19	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	19	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	19	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	19	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	19	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	19	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	19	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	19	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	19	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	19	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	19	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	19	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	19	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	19	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	19	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	19	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	19	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	19	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	19	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	19	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	19	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	19	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	19	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	19	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG12	20	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG13	20	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG21	20	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG22	20	0.65
(1,2606)	1:84:B:VAL:HG11	1:84:B:VAL:HG23	20	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG11	20	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG13	20	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG21	20	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG22	20	0.65
(1,2606)	1:84:B:VAL:HG12	1:84:B:VAL:HG23	20	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG11	20	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG12	20	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG21	20	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG22	20	0.65
(1,2606)	1:84:B:VAL:HG13	1:84:B:VAL:HG23	20	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG11	20	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG12	20	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG13	20	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG22	20	0.65
(1,2606)	1:84:B:VAL:HG21	1:84:B:VAL:HG23	20	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG11	20	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG12	20	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG13	20	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG21	20	0.65
(1,2606)	1:84:B:VAL:HG22	1:84:B:VAL:HG23	20	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG11	20	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG12	20	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG13	20	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG21	20	0.65
(1,2606)	1:84:B:VAL:HG23	1:84:B:VAL:HG22	20	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	1	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	1	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	1	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	1	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	1	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	1	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	1	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	1	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	1	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	1	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	1	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	1	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	1	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	1	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	1	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	1	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	1	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	1	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	1	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	1	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	1	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	1	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	1	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	1	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	1	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	1	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	1	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	1	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	1	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	2	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	2	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	2	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	2	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	2	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	2	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	2	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	2	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	2	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	2	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	2	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	2	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	2	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	2	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	2	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	2	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	2	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	2	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	2	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	2	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	2	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	2	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	2	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	2	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	2	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	2	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	2	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	2	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	2	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	3	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	3	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	3	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	3	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	3	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	3	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	3	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	3	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	3	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	3	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	3	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	3	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	3	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	3	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	3	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	3	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	3	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	3	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	3	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	3	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	3	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	3	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	3	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	3	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	3	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	3	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	3	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	3	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	3	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	4	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	4	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	4	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	4	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	4	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	4	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	4	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	4	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	4	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	4	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	4	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	4	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	4	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	4	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	4	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	4	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	4	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	4	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	4	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	4	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	4	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	4	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	4	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	4	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	4	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	4	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	4	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	4	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	4	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	4	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	5	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	5	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	5	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	5	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	5	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	5	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	5	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	5	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	5	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	5	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	5	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	5	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	5	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	5	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	5	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	5	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	5	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	5	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	5	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	5	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	5	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	5	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	5	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	5	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	5	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	5	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	5	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	5	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	5	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	6	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	6	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	6	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	6	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	6	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	6	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	6	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	6	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	6	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	6	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	6	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	6	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	6	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	6	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	6	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	6	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	6	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	6	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	6	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	6	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	6	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	6	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	6	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	6	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	6	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	6	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	6	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	6	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	6	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	7	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	7	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	7	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	7	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	7	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	7	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	7	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	7	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	7	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	7	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	7	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	7	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	7	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	7	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	7	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	7	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	7	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	7	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	7	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	7	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	7	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	7	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	7	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	7	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	7	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	7	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	7	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	7	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	7	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	7	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	8	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	8	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	8	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	8	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	8	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	8	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	8	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	8	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	8	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	8	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	8	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	8	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	8	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	8	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	8	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	8	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	8	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	8	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	8	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	8	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	8	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	8	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	8	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	8	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	8	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	8	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	8	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	8	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	8	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	9	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	9	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	9	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	9	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	9	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	9	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	9	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	9	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	9	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	9	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	9	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	9	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	9	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	9	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	9	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	9	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	9	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	9	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	9	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	9	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	9	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	9	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	9	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	9	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	9	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	9	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	9	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	9	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	9	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	10	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	10	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	10	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	10	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	10	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	10	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	10	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	10	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	10	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	10	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	10	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	10	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	10	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	10	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	10	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	10	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	10	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	10	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	10	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	10	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	10	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	10	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	10	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	10	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	10	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	10	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	10	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	10	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	10	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	11	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	11	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	11	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	11	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	11	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	11	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	11	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	11	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	11	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	11	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	11	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	11	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	11	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	11	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	11	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	11	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	11	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	11	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	11	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	11	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	11	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	11	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	11	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	11	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	11	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	11	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	11	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	11	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	11	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	11	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	12	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	12	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	12	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	12	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	12	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	12	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	12	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	12	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	12	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	12	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	12	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	12	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	12	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	12	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	12	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	12	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	12	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	12	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	12	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	12	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	12	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	12	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	12	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	12	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	12	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	12	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	12	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	12	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	12	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	13	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	13	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	13	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	13	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	13	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	13	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	13	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	13	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	13	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	13	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	13	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	13	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	13	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	13	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	13	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	13	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	13	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	13	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	13	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	13	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	13	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	13	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	13	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	13	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	13	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	13	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	13	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	13	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	13	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	14	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	14	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	14	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	14	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	14	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	14	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	14	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	14	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	14	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	14	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	14	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	14	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	14	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	14	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	14	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	14	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	14	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	14	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	14	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	14	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	14	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	14	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	14	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	14	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	14	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	14	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	14	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	14	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	14	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	14	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	15	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	15	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	15	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	15	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	15	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	15	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	15	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	15	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	15	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	15	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	15	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	15	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	15	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	15	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	15	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	15	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	15	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	15	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	15	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	15	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	15	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	15	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	15	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	15	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	15	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	15	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	15	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	15	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	15	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	16	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	16	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	16	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	16	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	16	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	16	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	16	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	16	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	16	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	16	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	16	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	16	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	16	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	16	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	16	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	16	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	16	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	16	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	16	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	16	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	16	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	16	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	16	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	16	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	16	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	16	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	16	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	16	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	16	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	17	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	17	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	17	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	17	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	17	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	17	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	17	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	17	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	17	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	17	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	17	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	17	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	17	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	17	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	17	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	17	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	17	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	17	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	17	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	17	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	17	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	17	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	17	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	17	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	17	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	17	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	17	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	17	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	17	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	18	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	18	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	18	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	18	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	18	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	18	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	18	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	18	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	18	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	18	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	18	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	18	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	18	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	18	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	18	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	18	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	18	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	18	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	18	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	18	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	18	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	18	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	18	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	18	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	18	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	18	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	18	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	18	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	18	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	18	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	19	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	19	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	19	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	19	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	19	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	19	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	19	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	19	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	19	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	19	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	19	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	19	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	19	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	19	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	19	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	19	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	19	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	19	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	19	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	19	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	19	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	19	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	19	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	19	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	19	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	19	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	19	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	19	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	19	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG12	20	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG13	20	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG21	20	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG22	20	0.65
(1,2304)	1:37:B:VAL:HG11	1:37:B:VAL:HG23	20	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG11	20	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG13	20	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG21	20	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG22	20	0.65
(1,2304)	1:37:B:VAL:HG12	1:37:B:VAL:HG23	20	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG11	20	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG12	20	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG21	20	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG22	20	0.65
(1,2304)	1:37:B:VAL:HG13	1:37:B:VAL:HG23	20	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG11	20	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG12	20	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG13	20	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG22	20	0.65
(1,2304)	1:37:B:VAL:HG21	1:37:B:VAL:HG23	20	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG11	20	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG12	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG13	20	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG21	20	0.65
(1,2304)	1:37:B:VAL:HG22	1:37:B:VAL:HG23	20	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG11	20	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG12	20	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG13	20	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG21	20	0.65
(1,2304)	1:37:B:VAL:HG23	1:37:B:VAL:HG22	20	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	1	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	1	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	1	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	1	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	1	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	1	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	1	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	1	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	1	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	1	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	1	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	1	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	1	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	1	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	1	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	1	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	1	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	1	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	1	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	1	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	1	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	1	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	1	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	1	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	1	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	1	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	1	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	1	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	1	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	1	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	2	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	2	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	2	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	2	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	2	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	2	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	2	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	2	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	2	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	2	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	2	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	2	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	2	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	2	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	2	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	2	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	2	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	2	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	2	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	2	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	2	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	2	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	2	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	2	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	2	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	2	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	2	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	2	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	2	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	3	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	3	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	3	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	3	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	3	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	3	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	3	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	3	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	3	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	3	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	3	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	3	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	3	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	3	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	3	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	3	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	3	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	3	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	3	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	3	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	3	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	3	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	3	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	3	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	3	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	3	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	3	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	3	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	3	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	4	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	4	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	4	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	4	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	4	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	4	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	4	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	4	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	4	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	4	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	4	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	4	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	4	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	4	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	4	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	4	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	4	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	4	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	4	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	4	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	4	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	4	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	4	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	4	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	4	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	4	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	4	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	4	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	4	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	5	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	5	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	5	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	5	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	5	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	5	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	5	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	5	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	5	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	5	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	5	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	5	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	5	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	5	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	5	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	5	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	5	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	5	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	5	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	5	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	5	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	5	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	5	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	5	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	5	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	5	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	5	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	5	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	5	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	5	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	6	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	6	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	6	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	6	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	6	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	6	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	6	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	6	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	6	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	6	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	6	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	6	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	6	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	6	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	6	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	6	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	6	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	6	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	6	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	6	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	6	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	6	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	6	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	6	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	6	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	6	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	6	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	6	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	6	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	7	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	7	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	7	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	7	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	7	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	7	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	7	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	7	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	7	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	7	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	7	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	7	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	7	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	7	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	7	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	7	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	7	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	7	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	7	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	7	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	7	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	7	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	7	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	7	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	7	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	7	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	7	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	7	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	7	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	8	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	8	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	8	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	8	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	8	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	8	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	8	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	8	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	8	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	8	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	8	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	8	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	8	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	8	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	8	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	8	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	8	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	8	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	8	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	8	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	8	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	8	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	8	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	8	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	8	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	8	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	8	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	8	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	8	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	8	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	9	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	9	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	9	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	9	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	9	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	9	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	9	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	9	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	9	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	9	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	9	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	9	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	9	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	9	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	9	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	9	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	9	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	9	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	9	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	9	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	9	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	9	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	9	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	9	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	9	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	9	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	9	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	9	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	9	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	10	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	10	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	10	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	10	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	10	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	10	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	10	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	10	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	10	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	10	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	10	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	10	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	10	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	10	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	10	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	10	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	10	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	10	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	10	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	10	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	10	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	10	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	10	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	10	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	10	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	10	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	10	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	10	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	10	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	11	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	11	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	11	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	11	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	11	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	11	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	11	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	11	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	11	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	11	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	11	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	11	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	11	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	11	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	11	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	11	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	11	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	11	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	11	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	11	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	11	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	11	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	11	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	11	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	11	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	11	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	11	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	11	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	11	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	12	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	12	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	12	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	12	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	12	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	12	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	12	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	12	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	12	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	12	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	12	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	12	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	12	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	12	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	12	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	12	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	12	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	12	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	12	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	12	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	12	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	12	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	12	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	12	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	12	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	12	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	12	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	12	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	12	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	12	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	13	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	13	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	13	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	13	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	13	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	13	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	13	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	13	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	13	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	13	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	13	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	13	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	13	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	13	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	13	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	13	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	13	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	13	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	13	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	13	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	13	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	13	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	13	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	13	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	13	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	13	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	13	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	13	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	13	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	14	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	14	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	14	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	14	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	14	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	14	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	14	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	14	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	14	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	14	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	14	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	14	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	14	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	14	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	14	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	14	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	14	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	14	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	14	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	14	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	14	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	14	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	14	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	14	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	14	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	14	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	14	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	14	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	14	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	15	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	15	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	15	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	15	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	15	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	15	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	15	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	15	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	15	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	15	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	15	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	15	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	15	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	15	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	15	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	15	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	15	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	15	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	15	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	15	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	15	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	15	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	15	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	15	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	15	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	15	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	15	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	15	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	15	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	15	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	16	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	16	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	16	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	16	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	16	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	16	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	16	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	16	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	16	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	16	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	16	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	16	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	16	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	16	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	16	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	16	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	16	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	16	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	16	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	16	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	16	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	16	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	16	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	16	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	16	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	16	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	16	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	16	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	16	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	17	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	17	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	17	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	17	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	17	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	17	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	17	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	17	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	17	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	17	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	17	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	17	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	17	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	17	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	17	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	17	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	17	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	17	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	17	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	17	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	17	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	17	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	17	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	17	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	17	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	17	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	17	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	17	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	17	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	18	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	18	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	18	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	18	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	18	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	18	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	18	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	18	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	18	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	18	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	18	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	18	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	18	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	18	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	18	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	18	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	18	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	18	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	18	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	18	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	18	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	18	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	18	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	18	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	18	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	18	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	18	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	18	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	18	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	19	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	19	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	19	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	19	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	19	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	19	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	19	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	19	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	19	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	19	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	19	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	19	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	19	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	19	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	19	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	19	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	19	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	19	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	19	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	19	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	19	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	19	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	19	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	19	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	19	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	19	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	19	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	19	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	19	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	19	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	20	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	20	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	20	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	20	0.65
(1,2229)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	20	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	20	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	20	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	20	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	20	0.65
(1,2229)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	20	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	20	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	20	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	20	0.65
(1,2229)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	20	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	20	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	20	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	20	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	20	0.65
(1,2229)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	20	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	20	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	20	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	20	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	20	0.65
(1,2229)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	20	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	20	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	20	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	20	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	20	0.65
(1,2229)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	20	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	1	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	1	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	1	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	1	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	1	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	1	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	1	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	1	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	1	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	1	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	1	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	1	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	1	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	1	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	1	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	1	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	1	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	1	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	1	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	1	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	1	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	1	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	1	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	1	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	1	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	1	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	1	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	1	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	1	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	2	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	2	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	2	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	2	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	2	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	2	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	2	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	2	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	2	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	2	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	2	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	2	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	2	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	2	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	2	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	2	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	2	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	2	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	2	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	2	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	2	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	2	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	2	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	2	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	2	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	2	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	2	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	2	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	2	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	2	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	3	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	3	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	3	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	3	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	3	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	3	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	3	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	3	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	3	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	3	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	3	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	3	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	3	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	3	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	3	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	3	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	3	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	3	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	3	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	3	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	3	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	3	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	3	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	3	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	3	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	3	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	3	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	3	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	3	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	4	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	4	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	4	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	4	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	4	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	4	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	4	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	4	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	4	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	4	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	4	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	4	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	4	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	4	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	4	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	4	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	4	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	4	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	4	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	4	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	4	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	4	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	4	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	4	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	4	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	4	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	4	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	4	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	4	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	5	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	5	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	5	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	5	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	5	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	5	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	5	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	5	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	5	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	5	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	5	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	5	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	5	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	5	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	5	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	5	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	5	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	5	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	5	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	5	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	5	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	5	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	5	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	5	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	5	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	5	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	5	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	5	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	5	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	6	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	6	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	6	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	6	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	6	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	6	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	6	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	6	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	6	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	6	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	6	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	6	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	6	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	6	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	6	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	6	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	6	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	6	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	6	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	6	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	6	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	6	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	6	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	6	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	6	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	6	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	6	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	6	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	6	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	6	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	7	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	7	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	7	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	7	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	7	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	7	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	7	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	7	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	7	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	7	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	7	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	7	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	7	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	7	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	7	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	7	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	7	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	7	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	7	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	7	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	7	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	7	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	7	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	7	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	7	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	7	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	7	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	7	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	7	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	8	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	8	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	8	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	8	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	8	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	8	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	8	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	8	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	8	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	8	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	8	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	8	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	8	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	8	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	8	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	8	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	8	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	8	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	8	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	8	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	8	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	8	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	8	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	8	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	8	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	8	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	8	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	8	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	8	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	9	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	9	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	9	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	9	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	9	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	9	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	9	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	9	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	9	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	9	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	9	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	9	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	9	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	9	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	9	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	9	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	9	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	9	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	9	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	9	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	9	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	9	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	9	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	9	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	9	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	9	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	9	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	9	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	9	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	9	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	10	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	10	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	10	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	10	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	10	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	10	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	10	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	10	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	10	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	10	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	10	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	10	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	10	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	10	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	10	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	10	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	10	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	10	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	10	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	10	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	10	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	10	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	10	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	10	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	10	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	10	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	10	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	10	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	10	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	11	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	11	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	11	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	11	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	11	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	11	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	11	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	11	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	11	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	11	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	11	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	11	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	11	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	11	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	11	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	11	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	11	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	11	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	11	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	11	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	11	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	11	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	11	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	11	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	11	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	11	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	11	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	11	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	11	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	12	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	12	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	12	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	12	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	12	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	12	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	12	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	12	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	12	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	12	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	12	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	12	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	12	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	12	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	12	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	12	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	12	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	12	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	12	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	12	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	12	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	12	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	12	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	12	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	12	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	12	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	12	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	12	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	12	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	13	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	13	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	13	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	13	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	13	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	13	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	13	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	13	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	13	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	13	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	13	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	13	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	13	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	13	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	13	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	13	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	13	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	13	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	13	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	13	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	13	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	13	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	13	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	13	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	13	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	13	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	13	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	13	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	13	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	13	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	14	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	14	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	14	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	14	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	14	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	14	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	14	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	14	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	14	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	14	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	14	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	14	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	14	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	14	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	14	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	14	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	14	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	14	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	14	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	14	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	14	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	14	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	14	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	14	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	14	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	14	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	14	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	14	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	14	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	15	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	15	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	15	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	15	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	15	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	15	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	15	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	15	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	15	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	15	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	15	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	15	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	15	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	15	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	15	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	15	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	15	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	15	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	15	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	15	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	15	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	15	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	15	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	15	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	15	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	15	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	15	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	15	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	15	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	16	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	16	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	16	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	16	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	16	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	16	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	16	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	16	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	16	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	16	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	16	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	16	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	16	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	16	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	16	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	16	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	16	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	16	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	16	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	16	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	16	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	16	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	16	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	16	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	16	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	16	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	16	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	16	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	16	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	16	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	17	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	17	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	17	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	17	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	17	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	17	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	17	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	17	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	17	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	17	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	17	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	17	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	17	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	17	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	17	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	17	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	17	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	17	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	17	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	17	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	17	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	17	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	17	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	17	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	17	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	17	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	17	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	17	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	17	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	18	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	18	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	18	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	18	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	18	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	18	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	18	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	18	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	18	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	18	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	18	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	18	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	18	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	18	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	18	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	18	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	18	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	18	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	18	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	18	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	18	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	18	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	18	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	18	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	18	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	18	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	18	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	18	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	18	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	19	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	19	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	19	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	19	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	19	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	19	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	19	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	19	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	19	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	19	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	19	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	19	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	19	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	19	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	19	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	19	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	19	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	19	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	19	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	19	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	19	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	19	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	19	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	19	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	19	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	19	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	19	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	19	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	19	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG12	20	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG13	20	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG21	20	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG22	20	0.65
(1,2228)	1:24:B:VAL:HG11	1:24:B:VAL:HG23	20	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG11	20	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG13	20	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG21	20	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG22	20	0.65
(1,2228)	1:24:B:VAL:HG12	1:24:B:VAL:HG23	20	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG11	20	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG12	20	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG21	20	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG22	20	0.65
(1,2228)	1:24:B:VAL:HG13	1:24:B:VAL:HG23	20	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG11	20	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG12	20	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG13	20	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG22	20	0.65
(1,2228)	1:24:B:VAL:HG21	1:24:B:VAL:HG23	20	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG11	20	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG12	20	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG13	20	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG21	20	0.65
(1,2228)	1:24:B:VAL:HG22	1:24:B:VAL:HG23	20	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG11	20	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG12	20	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG13	20	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG21	20	0.65
(1,2228)	1:24:B:VAL:HG23	1:24:B:VAL:HG22	20	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	1	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	1	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	1	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	1	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	1	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	1	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	1	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	1	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	1	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	1	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	1	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	1	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	1	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	1	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	1	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	1	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	1	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	1	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	1	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	1	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	1	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	1	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	1	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	1	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	1	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	1	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	1	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	1	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	1	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	2	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	2	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	2	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	2	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	2	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	2	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	2	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	2	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	2	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	2	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	2	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	2	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	2	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	2	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	2	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	2	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	2	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	2	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	2	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	2	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	2	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	2	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	2	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	2	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	2	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	2	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	2	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	2	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	2	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	3	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	3	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	3	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	3	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	3	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	3	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	3	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	3	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	3	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	3	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	3	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	3	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	3	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	3	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	3	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	3	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	3	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	3	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	3	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	3	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	3	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	3	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	3	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	3	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	3	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	3	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	3	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	3	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	3	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	3	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	4	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	4	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	4	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	4	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	4	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	4	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	4	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	4	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	4	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	4	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	4	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	4	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	4	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	4	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	4	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	4	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	4	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	4	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	4	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	4	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	4	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	4	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	4	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	4	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	4	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	4	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	4	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	4	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	4	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	5	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	5	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	5	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	5	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	5	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	5	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	5	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	5	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	5	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	5	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	5	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	5	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	5	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	5	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	5	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	5	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	5	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	5	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	5	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	5	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	5	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	5	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	5	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	5	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	5	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	5	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	5	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	5	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	5	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	6	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	6	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	6	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	6	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	6	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	6	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	6	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	6	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	6	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	6	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	6	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	6	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	6	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	6	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	6	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	6	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	6	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	6	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	6	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	6	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	6	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	6	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	6	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	6	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	6	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	6	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	6	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	6	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	6	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	7	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	7	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	7	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	7	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	7	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	7	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	7	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	7	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	7	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	7	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	7	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	7	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	7	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	7	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	7	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	7	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	7	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	7	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	7	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	7	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	7	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	7	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	7	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	7	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	7	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	7	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	7	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	7	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	7	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	7	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	8	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	8	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	8	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	8	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	8	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	8	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	8	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	8	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	8	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	8	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	8	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	8	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	8	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	8	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	8	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	8	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	8	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	8	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	8	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	8	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	8	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	8	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	8	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	8	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	8	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	8	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	8	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	8	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	8	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	9	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	9	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	9	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	9	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	9	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	9	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	9	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	9	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	9	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	9	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	9	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	9	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	9	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	9	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	9	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	9	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	9	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	9	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	9	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	9	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	9	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	9	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	9	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	9	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	9	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	9	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	9	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	9	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	9	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	10	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	10	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	10	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	10	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	10	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	10	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	10	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	10	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	10	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	10	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	10	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	10	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	10	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	10	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	10	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	10	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	10	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	10	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	10	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	10	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	10	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	10	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	10	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	10	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	10	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	10	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	10	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	10	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	10	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	10	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	11	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	11	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	11	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	11	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	11	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	11	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	11	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	11	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	11	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	11	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	11	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	11	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	11	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	11	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	11	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	11	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	11	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	11	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	11	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	11	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	11	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	11	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	11	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	11	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	11	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	11	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	11	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	11	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	11	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	12	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	12	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	12	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	12	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	12	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	12	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	12	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	12	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	12	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	12	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	12	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	12	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	12	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	12	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	12	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	12	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	12	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	12	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	12	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	12	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	12	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	12	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	12	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	12	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	12	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	12	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	12	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	12	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	12	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	13	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	13	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	13	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	13	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	13	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	13	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	13	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	13	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	13	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	13	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	13	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	13	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	13	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	13	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	13	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	13	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	13	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	13	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	13	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	13	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	13	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	13	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	13	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	13	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	13	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	13	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	13	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	13	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	13	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	14	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	14	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	14	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	14	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	14	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	14	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	14	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	14	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	14	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	14	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	14	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	14	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	14	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	14	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	14	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	14	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	14	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	14	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	14	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	14	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	14	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	14	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	14	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	14	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	14	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	14	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	14	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	14	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	14	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	14	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	15	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	15	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	15	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	15	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	15	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	15	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	15	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	15	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	15	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	15	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	15	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	15	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	15	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	15	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	15	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	15	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	15	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	15	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	15	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	15	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	15	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	15	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	15	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	15	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	15	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	15	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	15	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	15	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	15	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	16	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	16	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	16	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	16	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	16	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	16	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	16	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	16	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	16	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	16	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	16	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	16	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	16	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	16	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	16	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	16	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	16	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	16	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	16	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	16	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	16	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	16	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	16	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	16	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	16	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	16	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	16	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	16	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	16	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	17	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	17	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	17	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	17	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	17	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	17	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	17	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	17	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	17	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	17	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	17	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	17	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	17	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	17	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	17	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	17	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	17	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	17	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	17	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	17	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	17	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	17	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	17	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	17	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	17	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	17	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	17	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	17	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	17	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	17	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	18	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	18	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	18	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	18	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	18	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	18	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	18	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	18	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	18	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	18	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	18	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	18	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	18	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	18	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	18	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	18	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	18	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	18	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	18	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	18	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	18	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	18	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	18	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	18	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	18	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	18	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	18	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	18	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	18	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	19	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	19	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	19	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	19	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	19	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	19	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	19	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	19	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	19	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	19	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	19	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	19	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	19	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	19	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	19	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	19	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	19	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	19	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	19	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	19	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	19	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	19	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	19	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	19	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	19	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	19	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	19	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	19	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	19	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	20	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	20	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	20	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	20	0.65
(1,2135)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	20	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	20	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	20	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	20	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	20	0.65
(1,2135)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	20	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	20	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	20	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	20	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	20	0.65
(1,2135)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	20	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	20	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	20	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	20	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	20	0.65
(1,2135)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	20	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	20	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	20	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	20	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	20	0.65
(1,2135)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	20	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	20	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	20	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	20	0.65
(1,2135)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	20	0.65
(1,1959)	1:89:B:THR:HG23	1:87:B:LEU:HB2	3	0.65
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	3	0.65
(1,1720)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	2	0.65
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	15	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	1	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	1	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	1	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	1	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	1	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	1	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	1	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	1	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	1	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	1	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	1	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	1	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	1	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	1	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	1	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	1	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	1	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	1	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	1	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	1	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	1	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	1	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	1	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	1	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	1	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	1	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	1	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	1	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	1	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	1	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	2	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	2	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	2	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	2	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	2	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	2	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	2	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	2	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	2	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	2	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	2	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	2	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	2	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	2	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	2	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	2	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	2	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	2	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	2	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	2	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	2	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	2	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	2	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	2	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	2	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	2	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	2	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	2	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	2	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	3	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	3	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	3	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	3	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	3	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	3	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	3	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	3	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	3	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	3	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	3	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	3	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	3	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	3	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	3	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	3	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	3	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	3	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	3	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	3	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	3	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	3	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	3	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	3	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	3	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	3	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	3	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	3	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	3	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	4	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	4	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	4	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	4	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	4	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	4	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	4	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	4	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	4	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	4	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	4	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	4	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	4	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	4	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	4	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	4	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	4	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	4	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	4	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	4	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	4	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	4	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	4	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	4	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	4	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	4	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	4	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	4	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	4	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	5	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	5	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	5	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	5	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	5	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	5	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	5	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	5	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	5	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	5	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	5	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	5	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	5	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	5	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	5	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	5	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	5	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	5	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	5	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	5	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	5	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	5	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	5	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	5	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	5	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	5	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	5	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	5	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	5	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	5	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	6	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	6	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	6	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	6	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	6	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	6	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	6	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	6	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	6	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	6	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	6	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	6	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	6	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	6	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	6	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	6	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	6	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	6	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	6	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	6	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	6	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	6	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	6	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	6	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	6	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	6	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	6	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	6	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	6	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	7	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	7	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	7	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	7	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	7	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	7	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	7	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	7	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	7	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	7	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	7	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	7	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	7	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	7	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	7	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	7	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	7	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	7	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	7	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	7	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	7	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	7	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	7	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	7	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	7	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	7	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	7	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	7	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	7	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	8	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	8	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	8	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	8	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	8	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	8	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	8	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	8	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	8	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	8	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	8	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	8	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	8	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	8	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	8	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	8	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	8	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	8	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	8	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	8	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	8	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	8	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	8	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	8	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	8	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	8	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	8	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	8	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	8	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	8	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	9	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	9	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	9	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	9	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	9	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	9	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	9	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	9	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	9	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	9	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	9	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	9	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	9	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	9	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	9	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	9	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	9	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	9	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	9	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	9	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	9	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	9	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	9	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	9	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	9	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	9	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	9	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	9	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	9	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	10	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	10	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	10	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	10	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	10	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	10	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	10	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	10	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	10	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	10	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	10	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	10	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	10	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	10	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	10	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	10	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	10	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	10	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	10	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	10	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	10	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	10	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	10	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	10	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	10	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	10	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	10	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	10	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	10	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	11	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	11	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	11	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	11	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	11	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	11	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	11	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	11	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	11	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	11	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	11	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	11	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	11	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	11	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	11	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	11	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	11	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	11	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	11	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	11	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	11	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	11	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	11	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	11	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	11	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	11	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	11	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	11	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	11	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	12	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	12	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	12	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	12	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	12	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	12	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	12	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	12	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	12	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	12	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	12	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	12	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	12	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	12	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	12	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	12	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	12	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	12	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	12	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	12	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	12	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	12	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	12	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	12	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	12	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	12	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	12	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	12	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	12	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	12	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	13	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	13	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	13	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	13	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	13	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	13	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	13	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	13	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	13	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	13	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	13	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	13	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	13	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	13	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	13	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	13	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	13	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	13	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	13	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	13	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	13	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	13	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	13	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	13	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	13	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	13	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	13	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	13	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	13	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	14	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	14	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	14	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	14	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	14	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	14	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	14	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	14	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	14	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	14	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	14	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	14	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	14	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	14	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	14	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	14	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	14	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	14	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	14	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	14	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	14	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	14	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	14	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	14	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	14	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	14	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	14	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	14	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	14	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	15	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	15	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	15	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	15	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	15	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	15	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	15	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	15	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	15	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	15	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	15	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	15	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	15	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	15	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	15	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	15	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	15	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	15	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	15	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	15	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	15	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	15	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	15	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	15	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	15	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	15	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	15	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	15	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	15	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	15	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	16	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	16	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	16	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	16	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	16	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	16	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	16	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	16	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	16	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	16	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	16	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	16	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	16	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	16	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	16	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	16	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	16	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	16	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	16	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	16	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	16	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	16	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	16	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	16	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	16	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	16	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	16	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	16	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	16	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	17	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	17	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	17	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	17	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	17	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	17	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	17	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	17	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	17	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	17	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	17	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	17	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	17	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	17	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	17	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	17	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	17	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	17	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	17	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	17	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	17	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	17	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	17	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	17	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	17	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	17	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	17	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	17	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	17	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	18	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	18	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	18	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	18	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	18	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	18	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	18	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	18	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	18	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	18	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	18	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	18	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	18	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	18	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	18	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	18	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	18	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	18	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	18	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	18	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	18	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	18	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	18	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	18	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	18	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	18	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	18	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	18	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	18	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	19	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	19	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	19	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	19	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	19	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	19	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	19	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	19	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	19	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	19	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	19	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	19	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	19	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	19	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	19	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	19	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	19	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	19	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	19	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	19	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	19	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	19	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	19	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	19	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	19	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	19	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	19	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	19	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	19	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	19	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD12	20	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD13	20	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD21	20	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD22	20	0.65
(1,1410)	1:6:B:LEU:HD11	1:6:B:LEU:HD23	20	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD11	20	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD13	20	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD21	20	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD22	20	0.65
(1,1410)	1:6:B:LEU:HD12	1:6:B:LEU:HD23	20	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD11	20	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD12	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD21	20	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD22	20	0.65
(1,1410)	1:6:B:LEU:HD13	1:6:B:LEU:HD23	20	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD11	20	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD12	20	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD13	20	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD22	20	0.65
(1,1410)	1:6:B:LEU:HD21	1:6:B:LEU:HD23	20	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD11	20	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD12	20	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD13	20	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD21	20	0.65
(1,1410)	1:6:B:LEU:HD22	1:6:B:LEU:HD23	20	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD11	20	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD12	20	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD13	20	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD21	20	0.65
(1,1410)	1:6:B:LEU:HD23	1:6:B:LEU:HD22	20	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	1	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	1	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	1	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	1	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	1	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	1	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	1	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	1	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	1	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	1	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	1	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	1	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	1	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	1	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	1	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	1	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	1	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	1	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	1	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	1	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	1	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	1	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	1	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	1	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	1	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	1	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	1	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	1	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	1	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	2	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	2	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	2	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	2	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	2	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	2	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	2	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	2	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	2	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	2	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	2	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	2	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	2	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	2	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	2	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	2	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	2	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	2	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	2	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	2	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	2	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	2	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	2	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	2	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	2	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	2	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	2	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	2	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	2	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	2	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	3	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	3	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	3	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	3	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	3	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	3	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	3	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	3	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	3	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	3	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	3	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	3	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	3	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	3	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	3	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	3	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	3	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	3	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	3	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	3	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	3	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	3	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	3	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	3	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	3	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	3	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	3	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	3	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	3	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	4	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	4	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	4	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	4	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	4	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	4	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	4	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	4	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	4	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	4	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	4	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	4	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	4	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	4	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	4	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	4	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	4	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	4	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	4	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	4	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	4	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	4	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	4	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	4	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	4	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	4	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	4	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	4	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	4	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	5	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	5	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	5	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	5	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	5	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	5	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	5	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	5	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	5	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	5	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	5	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	5	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	5	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	5	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	5	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	5	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	5	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	5	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	5	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	5	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	5	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	5	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	5	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	5	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	5	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	5	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	5	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	5	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	5	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	6	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	6	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	6	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	6	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	6	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	6	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	6	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	6	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	6	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	6	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	6	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	6	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	6	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	6	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	6	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	6	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	6	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	6	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	6	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	6	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	6	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	6	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	6	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	6	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	6	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	6	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	6	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	6	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	6	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	6	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	7	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	7	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	7	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	7	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	7	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	7	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	7	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	7	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	7	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	7	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	7	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	7	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	7	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	7	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	7	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	7	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	7	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	7	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	7	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	7	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	7	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	7	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	7	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	7	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	7	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	7	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	7	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	7	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	7	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	8	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	8	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	8	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	8	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	8	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	8	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	8	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	8	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	8	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	8	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	8	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	8	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	8	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	8	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	8	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	8	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	8	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	8	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	8	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	8	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	8	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	8	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	8	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	8	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	8	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	8	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	8	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	8	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	8	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	9	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	9	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	9	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	9	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	9	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	9	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	9	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	9	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	9	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	9	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	9	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	9	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	9	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	9	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	9	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	9	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	9	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	9	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	9	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	9	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	9	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	9	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	9	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	9	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	9	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	9	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	9	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	9	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	9	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	9	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	10	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	10	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	10	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	10	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	10	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	10	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	10	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	10	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	10	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	10	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	10	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	10	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	10	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	10	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	10	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	10	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	10	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	10	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	10	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	10	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	10	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	10	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	10	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	10	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	10	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	10	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	10	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	10	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	10	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	11	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	11	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	11	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	11	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	11	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	11	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	11	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	11	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	11	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	11	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	11	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	11	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	11	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	11	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	11	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	11	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	11	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	11	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	11	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	11	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	11	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	11	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	11	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	11	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	11	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	11	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	11	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	11	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	11	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	12	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	12	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	12	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	12	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	12	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	12	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	12	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	12	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	12	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	12	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	12	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	12	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	12	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	12	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	12	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	12	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	12	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	12	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	12	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	12	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	12	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	12	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	12	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	12	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	12	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	12	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	12	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	12	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	12	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	13	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	13	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	13	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	13	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	13	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	13	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	13	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	13	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	13	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	13	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	13	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	13	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	13	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	13	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	13	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	13	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	13	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	13	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	13	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	13	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	13	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	13	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	13	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	13	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	13	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	13	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	13	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	13	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	13	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	13	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	14	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	14	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	14	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	14	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	14	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	14	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	14	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	14	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	14	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	14	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	14	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	14	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	14	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	14	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	14	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	14	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	14	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	14	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	14	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	14	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	14	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	14	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	14	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	14	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	14	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	14	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	14	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	14	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	14	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	15	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	15	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	15	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	15	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	15	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	15	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	15	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	15	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	15	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	15	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	15	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	15	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	15	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	15	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	15	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	15	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	15	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	15	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	15	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	15	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	15	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	15	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	15	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	15	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	15	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	15	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	15	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	15	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	15	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	16	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	16	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	16	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	16	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	16	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	16	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	16	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	16	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	16	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	16	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	16	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	16	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	16	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	16	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	16	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	16	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	16	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	16	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	16	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	16	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	16	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	16	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	16	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	16	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	16	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	16	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	16	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	16	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	16	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	16	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	17	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	17	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	17	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	17	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	17	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	17	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	17	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	17	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	17	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	17	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	17	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	17	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	17	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	17	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	17	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	17	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	17	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	17	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	17	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	17	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	17	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	17	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	17	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	17	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	17	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	17	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	17	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	17	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	17	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	18	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	18	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	18	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	18	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	18	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	18	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	18	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	18	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	18	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	18	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	18	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	18	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	18	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	18	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	18	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	18	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	18	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	18	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	18	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	18	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	18	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	18	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	18	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	18	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	18	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	18	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	18	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	18	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	18	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	19	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	19	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	19	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	19	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	19	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	19	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	19	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	19	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	19	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	19	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	19	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	19	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	19	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	19	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	19	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	19	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	19	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	19	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	19	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	19	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	19	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	19	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	19	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	19	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	19	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	19	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	19	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	19	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	19	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD12	20	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD13	20	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD21	20	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD22	20	0.65
(1,1348)	1:101:A:LEU:HD11	1:101:A:LEU:HD23	20	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD11	20	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD13	20	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD21	20	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD22	20	0.65
(1,1348)	1:101:A:LEU:HD12	1:101:A:LEU:HD23	20	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD11	20	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD12	20	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD21	20	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD22	20	0.65
(1,1348)	1:101:A:LEU:HD13	1:101:A:LEU:HD23	20	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD11	20	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD12	20	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD13	20	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD22	20	0.65
(1,1348)	1:101:A:LEU:HD21	1:101:A:LEU:HD23	20	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD11	20	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD12	20	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD13	20	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD21	20	0.65
(1,1348)	1:101:A:LEU:HD22	1:101:A:LEU:HD23	20	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD11	20	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD12	20	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD13	20	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD21	20	0.65
(1,1348)	1:101:A:LEU:HD23	1:101:A:LEU:HD22	20	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	1	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	1	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	1	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	1	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	1	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	1	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	1	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	1	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	1	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	1	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	1	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	1	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	1	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	1	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	1	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	1	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	1	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	1	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	1	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	1	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	1	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	1	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	1	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	1	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	1	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	1	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	1	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	1	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	1	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	2	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	2	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	2	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	2	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	2	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	2	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	2	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	2	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	2	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	2	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	2	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	2	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	2	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	2	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	2	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	2	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	2	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	2	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	2	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	2	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	2	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	2	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	2	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	2	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	2	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	2	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	2	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	2	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	2	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	3	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	3	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	3	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	3	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	3	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	3	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	3	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	3	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	3	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	3	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	3	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	3	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	3	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	3	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	3	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	3	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	3	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	3	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	3	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	3	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	3	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	3	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	3	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	3	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	3	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	3	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	3	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	3	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	3	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	3	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	4	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	4	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	4	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	4	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	4	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	4	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	4	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	4	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	4	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	4	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	4	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	4	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	4	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	4	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	4	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	4	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	4	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	4	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	4	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	4	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	4	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	4	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	4	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	4	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	4	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	4	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	4	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	4	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	4	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	5	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	5	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	5	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	5	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	5	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	5	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	5	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	5	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	5	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	5	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	5	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	5	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	5	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	5	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	5	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	5	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	5	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	5	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	5	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	5	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	5	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	5	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	5	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	5	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	5	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	5	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	5	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	5	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	5	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	6	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	6	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	6	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	6	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	6	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	6	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	6	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	6	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	6	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	6	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	6	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	6	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	6	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	6	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	6	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	6	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	6	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	6	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	6	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	6	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	6	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	6	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	6	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	6	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	6	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	6	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	6	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	6	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	6	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	7	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	7	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	7	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	7	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	7	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	7	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	7	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	7	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	7	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	7	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	7	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	7	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	7	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	7	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	7	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	7	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	7	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	7	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	7	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	7	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	7	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	7	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	7	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	7	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	7	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	7	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	7	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	7	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	7	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	7	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	8	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	8	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	8	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	8	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	8	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	8	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	8	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	8	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	8	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	8	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	8	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	8	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	8	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	8	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	8	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	8	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	8	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	8	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	8	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	8	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	8	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	8	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	8	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	8	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	8	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	8	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	8	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	8	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	8	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	9	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	9	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	9	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	9	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	9	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	9	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	9	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	9	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	9	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	9	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	9	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	9	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	9	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	9	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	9	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	9	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	9	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	9	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	9	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	9	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	9	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	9	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	9	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	9	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	9	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	9	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	9	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	9	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	9	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	10	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	10	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	10	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	10	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	10	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	10	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	10	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	10	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	10	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	10	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	10	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	10	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	10	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	10	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	10	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	10	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	10	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	10	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	10	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	10	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	10	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	10	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	10	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	10	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	10	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	10	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	10	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	10	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	10	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	10	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	11	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	11	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	11	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	11	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	11	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	11	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	11	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	11	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	11	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	11	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	11	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	11	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	11	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	11	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	11	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	11	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	11	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	11	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	11	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	11	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	11	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	11	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	11	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	11	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	11	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	11	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	11	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	11	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	11	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	12	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	12	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	12	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	12	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	12	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	12	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	12	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	12	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	12	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	12	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	12	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	12	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	12	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	12	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	12	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	12	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	12	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	12	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	12	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	12	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	12	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	12	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	12	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	12	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	12	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	12	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	12	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	12	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	12	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	13	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	13	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	13	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	13	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	13	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	13	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	13	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	13	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	13	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	13	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	13	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	13	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	13	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	13	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	13	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	13	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	13	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	13	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	13	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	13	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	13	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	13	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	13	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	13	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	13	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	13	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	13	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	13	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	13	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	14	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	14	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	14	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	14	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	14	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	14	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	14	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	14	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	14	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	14	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	14	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	14	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	14	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	14	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	14	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	14	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	14	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	14	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	14	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	14	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	14	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	14	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	14	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	14	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	14	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	14	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	14	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	14	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	14	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	14	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	15	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	15	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	15	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	15	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	15	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	15	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	15	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	15	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	15	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	15	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	15	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	15	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	15	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	15	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	15	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	15	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	15	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	15	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	15	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	15	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	15	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	15	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	15	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	15	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	15	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	15	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	15	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	15	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	15	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	16	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	16	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	16	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	16	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	16	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	16	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	16	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	16	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	16	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	16	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	16	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	16	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	16	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	16	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	16	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	16	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	16	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	16	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	16	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	16	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	16	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	16	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	16	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	16	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	16	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	16	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	16	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	16	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	16	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	17	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	17	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	17	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	17	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	17	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	17	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	17	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	17	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	17	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	17	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	17	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	17	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	17	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	17	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	17	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	17	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	17	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	17	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	17	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	17	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	17	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	17	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	17	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	17	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	17	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	17	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	17	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	17	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	17	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	17	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	18	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	18	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	18	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	18	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	18	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	18	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	18	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	18	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	18	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	18	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	18	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	18	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	18	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	18	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	18	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	18	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	18	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	18	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	18	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	18	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	18	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	18	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	18	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	18	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	18	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	18	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	18	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	18	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	18	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	19	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	19	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	19	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	19	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	19	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	19	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	19	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	19	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	19	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	19	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	19	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	19	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	19	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	19	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	19	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	19	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	19	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	19	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	19	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	19	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	19	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	19	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	19	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	19	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	19	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	19	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	19	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	19	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	19	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	20	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	20	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	20	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	20	0.65
(1,1223)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	20	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	20	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	20	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	20	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	20	0.65
(1,1223)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	20	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	20	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	20	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	20	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	20	0.65
(1,1223)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	20	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	20	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	20	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	20	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	20	0.65
(1,1223)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	20	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	20	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	20	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	20	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	20	0.65
(1,1223)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	20	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	20	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	20	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	20	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	20	0.65
(1,1223)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	1	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	1	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	1	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	1	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	1	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	1	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	1	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	1	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	1	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	1	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	1	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	1	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	1	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	1	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	1	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	1	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	1	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	1	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	1	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	1	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	1	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	1	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	1	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	1	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	1	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	1	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	1	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	1	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	1	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	1	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	2	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	2	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	2	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	2	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	2	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	2	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	2	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	2	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	2	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	2	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	2	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	2	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	2	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	2	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	2	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	2	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	2	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	2	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	2	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	2	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	2	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	2	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	2	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	2	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	2	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	2	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	2	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	2	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	2	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	3	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	3	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	3	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	3	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	3	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	3	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	3	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	3	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	3	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	3	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	3	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	3	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	3	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	3	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	3	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	3	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	3	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	3	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	3	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	3	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	3	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	3	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	3	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	3	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	3	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	3	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	3	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	3	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	3	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	4	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	4	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	4	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	4	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	4	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	4	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	4	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	4	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	4	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	4	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	4	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	4	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	4	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	4	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	4	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	4	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	4	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	4	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	4	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	4	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	4	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	4	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	4	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	4	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	4	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	4	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	4	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	4	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	4	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	4	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	5	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	5	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	5	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	5	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	5	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	5	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	5	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	5	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	5	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	5	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	5	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	5	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	5	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	5	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	5	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	5	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	5	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	5	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	5	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	5	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	5	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	5	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	5	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	5	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	5	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	5	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	5	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	5	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	5	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	6	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	6	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	6	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	6	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	6	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	6	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	6	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	6	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	6	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	6	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	6	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	6	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	6	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	6	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	6	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	6	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	6	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	6	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	6	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	6	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	6	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	6	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	6	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	6	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	6	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	6	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	6	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	6	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	6	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	7	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	7	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	7	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	7	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	7	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	7	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	7	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	7	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	7	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	7	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	7	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	7	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	7	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	7	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	7	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	7	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	7	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	7	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	7	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	7	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	7	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	7	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	7	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	7	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	7	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	7	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	7	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	7	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	7	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	8	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	8	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	8	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	8	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	8	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	8	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	8	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	8	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	8	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	8	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	8	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	8	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	8	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	8	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	8	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	8	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	8	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	8	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	8	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	8	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	8	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	8	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	8	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	8	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	8	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	8	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	8	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	8	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	8	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	8	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	9	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	9	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	9	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	9	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	9	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	9	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	9	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	9	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	9	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	9	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	9	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	9	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	9	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	9	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	9	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	9	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	9	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	9	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	9	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	9	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	9	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	9	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	9	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	9	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	9	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	9	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	9	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	9	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	9	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	10	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	10	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	10	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	10	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	10	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	10	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	10	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	10	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	10	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	10	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	10	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	10	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	10	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	10	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	10	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	10	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	10	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	10	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	10	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	10	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	10	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	10	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	10	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	10	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	10	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	10	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	10	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	10	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	10	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	11	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	11	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	11	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	11	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	11	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	11	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	11	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	11	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	11	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	11	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	11	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	11	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	11	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	11	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	11	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	11	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	11	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	11	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	11	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	11	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	11	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	11	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	11	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	11	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	11	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	11	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	11	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	11	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	11	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	11	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	12	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	12	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	12	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	12	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	12	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	12	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	12	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	12	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	12	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	12	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	12	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	12	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	12	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	12	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	12	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	12	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	12	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	12	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	12	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	12	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	12	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	12	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	12	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	12	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	12	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	12	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	12	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	12	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	12	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	13	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	13	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	13	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	13	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	13	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	13	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	13	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	13	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	13	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	13	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	13	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	13	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	13	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	13	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	13	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	13	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	13	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	13	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	13	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	13	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	13	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	13	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	13	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	13	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	13	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	13	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	13	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	13	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	13	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	14	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	14	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	14	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	14	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	14	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	14	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	14	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	14	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	14	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	14	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	14	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	14	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	14	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	14	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	14	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	14	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	14	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	14	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	14	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	14	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	14	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	14	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	14	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	14	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	14	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	14	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	14	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	14	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	14	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	15	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	15	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	15	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	15	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	15	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	15	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	15	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	15	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	15	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	15	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	15	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	15	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	15	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	15	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	15	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	15	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	15	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	15	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	15	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	15	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	15	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	15	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	15	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	15	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	15	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	15	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	15	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	15	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	15	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	15	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	16	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	16	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	16	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	16	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	16	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	16	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	16	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	16	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	16	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	16	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	16	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	16	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	16	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	16	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	16	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	16	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	16	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	16	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	16	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	16	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	16	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	16	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	16	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	16	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	16	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	16	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	16	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	16	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	16	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	17	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	17	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	17	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	17	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	17	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	17	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	17	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	17	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	17	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	17	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	17	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	17	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	17	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	17	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	17	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	17	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	17	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	17	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	17	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	17	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	17	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	17	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	17	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	17	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	17	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	17	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	17	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	17	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	17	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	18	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	18	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	18	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	18	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	18	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	18	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	18	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	18	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	18	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	18	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	18	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	18	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	18	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	18	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	18	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	18	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	18	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	18	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	18	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	18	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	18	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	18	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	18	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	18	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	18	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	18	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	18	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	18	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	18	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	18	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	19	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	19	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	19	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	19	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	19	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	19	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	19	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	19	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	19	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	19	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	19	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	19	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	19	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	19	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	19	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	19	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	19	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	19	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	19	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	19	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	19	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	19	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	19	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	19	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	19	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	19	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	19	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	19	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	19	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG12	20	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG13	20	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG21	20	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG22	20	0.65
(1,1222)	1:84:A:VAL:HG11	1:84:A:VAL:HG23	20	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG11	20	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG13	20	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG21	20	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG22	20	0.65
(1,1222)	1:84:A:VAL:HG12	1:84:A:VAL:HG23	20	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG11	20	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG12	20	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG21	20	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG22	20	0.65
(1,1222)	1:84:A:VAL:HG13	1:84:A:VAL:HG23	20	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG11	20	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG12	20	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG13	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG22	20	0.65
(1,1222)	1:84:A:VAL:HG21	1:84:A:VAL:HG23	20	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG11	20	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG12	20	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG13	20	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG21	20	0.65
(1,1222)	1:84:A:VAL:HG22	1:84:A:VAL:HG23	20	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG11	20	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG12	20	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG13	20	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG21	20	0.65
(1,1222)	1:84:A:VAL:HG23	1:84:A:VAL:HG22	20	0.65
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	19	0.65
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	6	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	1	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	1	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	1	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	1	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	1	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	1	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	1	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	1	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	1	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	1	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	1	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	1	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	1	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	1	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	1	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	1	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	1	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	1	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	1	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	1	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	1	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	1	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	1	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	1	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	1	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	1	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	1	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	1	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	1	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	2	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	2	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	2	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	2	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	2	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	2	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	2	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	2	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	2	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	2	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	2	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	2	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	2	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	2	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	2	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	2	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	2	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	2	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	2	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	2	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	2	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	2	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	2	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	2	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	2	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	2	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	2	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	2	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	2	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	2	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	3	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	3	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	3	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	3	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	3	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	3	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	3	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	3	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	3	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	3	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	3	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	3	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	3	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	3	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	3	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	3	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	3	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	3	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	3	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	3	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	3	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	3	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	3	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	3	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	3	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	3	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	3	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	3	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	3	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	4	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	4	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	4	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	4	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	4	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	4	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	4	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	4	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	4	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	4	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	4	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	4	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	4	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	4	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	4	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	4	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	4	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	4	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	4	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	4	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	4	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	4	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	4	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	4	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	4	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	4	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	4	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	4	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	4	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	5	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	5	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	5	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	5	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	5	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	5	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	5	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	5	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	5	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	5	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	5	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	5	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	5	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	5	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	5	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	5	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	5	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	5	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	5	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	5	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	5	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	5	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	5	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	5	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	5	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	5	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	5	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	5	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	5	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	5	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	6	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	6	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	6	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	6	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	6	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	6	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	6	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	6	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	6	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	6	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	6	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	6	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	6	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	6	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	6	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	6	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	6	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	6	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	6	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	6	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	6	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	6	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	6	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	6	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	6	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	6	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	6	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	6	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	6	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	7	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	7	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	7	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	7	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	7	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	7	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	7	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	7	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	7	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	7	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	7	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	7	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	7	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	7	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	7	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	7	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	7	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	7	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	7	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	7	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	7	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	7	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	7	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	7	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	7	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	7	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	7	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	7	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	7	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	8	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	8	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	8	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	8	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	8	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	8	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	8	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	8	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	8	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	8	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	8	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	8	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	8	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	8	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	8	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	8	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	8	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	8	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	8	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	8	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	8	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	8	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	8	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	8	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	8	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	8	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	8	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	8	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	8	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	9	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	9	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	9	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	9	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	9	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	9	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	9	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	9	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	9	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	9	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	9	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	9	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	9	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	9	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	9	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	9	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	9	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	9	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	9	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	9	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	9	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	9	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	9	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	9	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	9	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	9	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	9	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	9	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	9	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	9	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	10	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	10	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	10	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	10	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	10	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	10	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	10	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	10	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	10	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	10	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	10	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	10	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	10	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	10	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	10	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	10	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	10	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	10	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	10	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	10	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	10	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	10	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	10	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	10	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	10	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	10	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	10	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	10	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	10	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	11	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	11	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	11	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	11	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	11	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	11	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	11	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	11	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	11	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	11	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	11	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	11	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	11	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	11	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	11	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	11	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	11	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	11	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	11	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	11	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	11	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	11	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	11	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	11	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	11	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	11	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	11	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	11	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	11	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	12	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	12	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	12	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	12	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	12	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	12	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	12	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	12	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	12	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	12	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	12	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	12	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	12	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	12	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	12	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	12	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	12	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	12	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	12	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	12	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	12	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	12	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	12	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	12	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	12	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	12	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	12	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	12	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	12	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	12	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	13	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	13	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	13	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	13	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	13	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	13	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	13	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	13	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	13	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	13	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	13	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	13	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	13	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	13	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	13	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	13	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	13	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	13	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	13	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	13	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	13	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	13	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	13	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	13	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	13	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	13	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	13	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	13	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	13	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	14	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	14	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	14	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	14	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	14	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	14	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	14	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	14	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	14	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	14	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	14	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	14	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	14	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	14	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	14	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	14	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	14	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	14	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	14	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	14	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	14	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	14	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	14	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	14	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	14	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	14	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	14	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	14	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	14	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	15	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	15	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	15	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	15	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	15	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	15	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	15	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	15	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	15	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	15	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	15	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	15	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	15	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	15	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	15	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	15	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	15	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	15	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	15	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	15	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	15	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	15	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	15	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	15	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	15	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	15	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	15	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	15	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	15	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	16	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	16	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	16	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	16	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	16	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	16	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	16	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	16	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	16	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	16	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	16	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	16	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	16	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	16	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	16	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	16	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	16	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	16	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	16	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	16	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	16	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	16	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	16	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	16	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	16	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	16	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	16	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	16	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	16	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	16	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	17	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	17	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	17	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	17	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	17	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	17	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	17	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	17	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	17	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	17	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	17	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	17	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	17	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	17	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	17	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	17	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	17	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	17	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	17	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	17	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	17	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	17	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	17	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	17	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	17	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	17	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	17	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	17	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	17	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	18	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	18	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	18	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	18	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	18	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	18	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	18	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	18	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	18	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	18	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	18	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	18	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	18	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	18	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	18	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	18	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	18	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	18	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	18	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	18	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	18	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	18	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	18	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	18	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	18	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	18	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	18	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	18	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	18	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	19	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	19	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	19	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	19	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	19	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	19	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	19	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	19	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	19	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	19	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	19	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	19	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	19	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	19	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	19	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	19	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	19	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	19	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	19	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	19	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	19	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	19	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	19	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	19	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	19	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	19	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	19	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	19	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	19	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	19	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG12	20	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG13	20	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG21	20	0.65
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG22	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,920)	1:37:A:VAL:HG11	1:37:A:VAL:HG23	20	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG11	20	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG13	20	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG21	20	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG22	20	0.65
(1,920)	1:37:A:VAL:HG12	1:37:A:VAL:HG23	20	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG11	20	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG12	20	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG21	20	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG22	20	0.65
(1,920)	1:37:A:VAL:HG13	1:37:A:VAL:HG23	20	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG11	20	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG12	20	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG13	20	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG22	20	0.65
(1,920)	1:37:A:VAL:HG21	1:37:A:VAL:HG23	20	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG11	20	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG12	20	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG13	20	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG21	20	0.65
(1,920)	1:37:A:VAL:HG22	1:37:A:VAL:HG23	20	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG11	20	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG12	20	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG13	20	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG21	20	0.65
(1,920)	1:37:A:VAL:HG23	1:37:A:VAL:HG22	20	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	1	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	1	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	1	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	1	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	1	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	1	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	1	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	1	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	1	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	1	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	1	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	1	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	1	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	1	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	1	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	1	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	1	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	1	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	1	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	1	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	1	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	1	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	1	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	1	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	1	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	1	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	1	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	1	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	1	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	2	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	2	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	2	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	2	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	2	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	2	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	2	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	2	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	2	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	2	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	2	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	2	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	2	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	2	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	2	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	2	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	2	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	2	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	2	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	2	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	2	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	2	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	2	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	2	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	2	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	2	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	2	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	2	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	2	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	3	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	3	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	3	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	3	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	3	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	3	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	3	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	3	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	3	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	3	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	3	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	3	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	3	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	3	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	3	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	3	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	3	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	3	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	3	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	3	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	3	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	3	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	3	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	3	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	3	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	3	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	3	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	3	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	3	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	3	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	4	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	4	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	4	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	4	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	4	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	4	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	4	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	4	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	4	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	4	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	4	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	4	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	4	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	4	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	4	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	4	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	4	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	4	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	4	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	4	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	4	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	4	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	4	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	4	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	4	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	4	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	4	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	4	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	4	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	5	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	5	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	5	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	5	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	5	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	5	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	5	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	5	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	5	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	5	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	5	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	5	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	5	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	5	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	5	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	5	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	5	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	5	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	5	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	5	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	5	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	5	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	5	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	5	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	5	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	5	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	5	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	5	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	5	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	6	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	6	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	6	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	6	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	6	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	6	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	6	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	6	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	6	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	6	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	6	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	6	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	6	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	6	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	6	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	6	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	6	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	6	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	6	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	6	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	6	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	6	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	6	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	6	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	6	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	6	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	6	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	6	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	6	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	6	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	7	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	7	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	7	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	7	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	7	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	7	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	7	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	7	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	7	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	7	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	7	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	7	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	7	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	7	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	7	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	7	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	7	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	7	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	7	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	7	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	7	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	7	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	7	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	7	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	7	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	7	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	7	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	7	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	7	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	8	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	8	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	8	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	8	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	8	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	8	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	8	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	8	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	8	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	8	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	8	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	8	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	8	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	8	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	8	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	8	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	8	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	8	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	8	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	8	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	8	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	8	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	8	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	8	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	8	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	8	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	8	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	8	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	8	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	9	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	9	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	9	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	9	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	9	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	9	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	9	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	9	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	9	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	9	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	9	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	9	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	9	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	9	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	9	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	9	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	9	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	9	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	9	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	9	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	9	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	9	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	9	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	9	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	9	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	9	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	9	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	9	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	9	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	10	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	10	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	10	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	10	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	10	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	10	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	10	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	10	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	10	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	10	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	10	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	10	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	10	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	10	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	10	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	10	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	10	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	10	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	10	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	10	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	10	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	10	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	10	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	10	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	10	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	10	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	10	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	10	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	10	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	10	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	11	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	11	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	11	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	11	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	11	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	11	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	11	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	11	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	11	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	11	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	11	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	11	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	11	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	11	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	11	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	11	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	11	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	11	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	11	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	11	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	11	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	11	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	11	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	11	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	11	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	11	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	11	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	11	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	11	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	12	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	12	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	12	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	12	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	12	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	12	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	12	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	12	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	12	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	12	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	12	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	12	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	12	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	12	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	12	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	12	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	12	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	12	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	12	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	12	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	12	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	12	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	12	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	12	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	12	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	12	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	12	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	12	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	12	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	13	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	13	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	13	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	13	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	13	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	13	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	13	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	13	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	13	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	13	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	13	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	13	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	13	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	13	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	13	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	13	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	13	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	13	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	13	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	13	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	13	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	13	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	13	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	13	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	13	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	13	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	13	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	13	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	13	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	13	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	14	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	14	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	14	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	14	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	14	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	14	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	14	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	14	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	14	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	14	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	14	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	14	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	14	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	14	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	14	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	14	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	14	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	14	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	14	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	14	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	14	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	14	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	14	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	14	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	14	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	14	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	14	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	14	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	14	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	15	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	15	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	15	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	15	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	15	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	15	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	15	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	15	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	15	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	15	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	15	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	15	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	15	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	15	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	15	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	15	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	15	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	15	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	15	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	15	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	15	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	15	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	15	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	15	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	15	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	15	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	15	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	15	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	15	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	16	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	16	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	16	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	16	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	16	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	16	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	16	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	16	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	16	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	16	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	16	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	16	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	16	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	16	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	16	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	16	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	16	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	16	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	16	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	16	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	16	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	16	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	16	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	16	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	16	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	16	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	16	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	16	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	16	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	17	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	17	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	17	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	17	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	17	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	17	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	17	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	17	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	17	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	17	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	17	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	17	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	17	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	17	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	17	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	17	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	17	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	17	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	17	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	17	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	17	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	17	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	17	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	17	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	17	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	17	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	17	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	17	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	17	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	17	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	18	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	18	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	18	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	18	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	18	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	18	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	18	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	18	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	18	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	18	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	18	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	18	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	18	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	18	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	18	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	18	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	18	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	18	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	18	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	18	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	18	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	18	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	18	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	18	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	18	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	18	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	18	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	18	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	18	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	19	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	19	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	19	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	19	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	19	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	19	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	19	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	19	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	19	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	19	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	19	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	19	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	19	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	19	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	19	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	19	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	19	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	19	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	19	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	19	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	19	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	19	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	19	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	19	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	19	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	19	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	19	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	19	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	19	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	20	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	20	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	20	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	20	0.65
(1,845)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	20	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	20	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	20	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	20	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	20	0.65
(1,845)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	20	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	20	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	20	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	20	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	20	0.65
(1,845)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	20	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	20	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	20	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	20	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	20	0.65
(1,845)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	20	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	20	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	20	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	20	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	20	0.65
(1,845)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	20	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	20	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	20	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	20	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	20	0.65
(1,845)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	20	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	1	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	1	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	1	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	1	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	1	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	1	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	1	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	1	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	1	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	1	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	1	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	1	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	1	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	1	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	1	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	1	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	1	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	1	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	1	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	1	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	1	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	1	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	1	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	1	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	1	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	1	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	1	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	1	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	1	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	2	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	2	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	2	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	2	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	2	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	2	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	2	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	2	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	2	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	2	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	2	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	2	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	2	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	2	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	2	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	2	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	2	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	2	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	2	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	2	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	2	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	2	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	2	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	2	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	2	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	2	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	2	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	2	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	2	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	3	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	3	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	3	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	3	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	3	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	3	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	3	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	3	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	3	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	3	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	3	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	3	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	3	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	3	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	3	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	3	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	3	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	3	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	3	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	3	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	3	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	3	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	3	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	3	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	3	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	3	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	3	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	3	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	3	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	4	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	4	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	4	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	4	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	4	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	4	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	4	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	4	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	4	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	4	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	4	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	4	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	4	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	4	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	4	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	4	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	4	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	4	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	4	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	4	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	4	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	4	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	4	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	4	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	4	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	4	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	4	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	4	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	4	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	4	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	5	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	5	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	5	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	5	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	5	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	5	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	5	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	5	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	5	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	5	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	5	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	5	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	5	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	5	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	5	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	5	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	5	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	5	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	5	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	5	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	5	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	5	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	5	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	5	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	5	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	5	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	5	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	5	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	5	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	6	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	6	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	6	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	6	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	6	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	6	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	6	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	6	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	6	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	6	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	6	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	6	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	6	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	6	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	6	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	6	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	6	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	6	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	6	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	6	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	6	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	6	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	6	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	6	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	6	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	6	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	6	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	6	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	6	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	7	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	7	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	7	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	7	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	7	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	7	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	7	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	7	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	7	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	7	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	7	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	7	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	7	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	7	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	7	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	7	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	7	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	7	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	7	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	7	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	7	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	7	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	7	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	7	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	7	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	7	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	7	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	7	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	7	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	7	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	8	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	8	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	8	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	8	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	8	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	8	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	8	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	8	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	8	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	8	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	8	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	8	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	8	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	8	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	8	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	8	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	8	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	8	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	8	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	8	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	8	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	8	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	8	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	8	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	8	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	8	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	8	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	8	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	8	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	9	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	9	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	9	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	9	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	9	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	9	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	9	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	9	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	9	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	9	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	9	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	9	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	9	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	9	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	9	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	9	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	9	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	9	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	9	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	9	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	9	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	9	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	9	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	9	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	9	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	9	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	9	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	9	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	9	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	10	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	10	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	10	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	10	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	10	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	10	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	10	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	10	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	10	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	10	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	10	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	10	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	10	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	10	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	10	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	10	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	10	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	10	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	10	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	10	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	10	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	10	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	10	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	10	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	10	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	10	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	10	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	10	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	10	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	11	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	11	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	11	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	11	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	11	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	11	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	11	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	11	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	11	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	11	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	11	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	11	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	11	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	11	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	11	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	11	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	11	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	11	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	11	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	11	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	11	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	11	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	11	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	11	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	11	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	11	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	11	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	11	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	11	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	11	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	12	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	12	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	12	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	12	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	12	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	12	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	12	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	12	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	12	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	12	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	12	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	12	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	12	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	12	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	12	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	12	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	12	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	12	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	12	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	12	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	12	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	12	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	12	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	12	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	12	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	12	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	12	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	12	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	12	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	13	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	13	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	13	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	13	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	13	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	13	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	13	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	13	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	13	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	13	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	13	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	13	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	13	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	13	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	13	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	13	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	13	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	13	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	13	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	13	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	13	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	13	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	13	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	13	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	13	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	13	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	13	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	13	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	13	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	14	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	14	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	14	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	14	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	14	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	14	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	14	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	14	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	14	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	14	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	14	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	14	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	14	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	14	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	14	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	14	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	14	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	14	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	14	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	14	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	14	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	14	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	14	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	14	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	14	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	14	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	14	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	14	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	14	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	14	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	15	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	15	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	15	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	15	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	15	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	15	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	15	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	15	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	15	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	15	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	15	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	15	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	15	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	15	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	15	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	15	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	15	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	15	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	15	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	15	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	15	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	15	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	15	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	15	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	15	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	15	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	15	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	15	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	15	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	16	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	16	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	16	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	16	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	16	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	16	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	16	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	16	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	16	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	16	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	16	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	16	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	16	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	16	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	16	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	16	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	16	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	16	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	16	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	16	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	16	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	16	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	16	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	16	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	16	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	16	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	16	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	16	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	16	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	17	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	17	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	17	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	17	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	17	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	17	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	17	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	17	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	17	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	17	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	17	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	17	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	17	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	17	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	17	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	17	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	17	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	17	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	17	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	17	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	17	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	17	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	17	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	17	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	17	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	17	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	17	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	17	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	17	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	18	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	18	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	18	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	18	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	18	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	18	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	18	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	18	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	18	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	18	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	18	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	18	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	18	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	18	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	18	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	18	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	18	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	18	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	18	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	18	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	18	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	18	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	18	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	18	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	18	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	18	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	18	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	18	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	18	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	18	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	19	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	19	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	19	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	19	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	19	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	19	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	19	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	19	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	19	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	19	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	19	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	19	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	19	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	19	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	19	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	19	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	19	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	19	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	19	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	19	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	19	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	19	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	19	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	19	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	19	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	19	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	19	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	19	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	19	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG12	20	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG13	20	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG21	20	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG22	20	0.65
(1,844)	1:24:A:VAL:HG11	1:24:A:VAL:HG23	20	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG11	20	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG13	20	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG21	20	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG22	20	0.65
(1,844)	1:24:A:VAL:HG12	1:24:A:VAL:HG23	20	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG11	20	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG12	20	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG21	20	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG22	20	0.65
(1,844)	1:24:A:VAL:HG13	1:24:A:VAL:HG23	20	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG11	20	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG12	20	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG13	20	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG22	20	0.65
(1,844)	1:24:A:VAL:HG21	1:24:A:VAL:HG23	20	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG11	20	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG12	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG13	20	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG21	20	0.65
(1,844)	1:24:A:VAL:HG22	1:24:A:VAL:HG23	20	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG11	20	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG12	20	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG13	20	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG21	20	0.65
(1,844)	1:24:A:VAL:HG23	1:24:A:VAL:HG22	20	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	1	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	1	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	1	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	1	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	1	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	1	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	1	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	1	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	1	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	1	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	1	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	1	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	1	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	1	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	1	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	1	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	1	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	1	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	1	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	1	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	1	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	1	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	1	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	1	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	1	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	1	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	1	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	1	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	1	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	1	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	2	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	2	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	2	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	2	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	2	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	2	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	2	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	2	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	2	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	2	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	2	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	2	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	2	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	2	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	2	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	2	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	2	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	2	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	2	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	2	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	2	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	2	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	2	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	2	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	2	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	2	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	2	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	2	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	2	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	3	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	3	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	3	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	3	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	3	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	3	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	3	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	3	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	3	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	3	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	3	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	3	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	3	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	3	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	3	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	3	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	3	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	3	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	3	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	3	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	3	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	3	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	3	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	3	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	3	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	3	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	3	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	3	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	3	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	3	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	4	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	4	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	4	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	4	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	4	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	4	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	4	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	4	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	4	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	4	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	4	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	4	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	4	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	4	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	4	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	4	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	4	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	4	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	4	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	4	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	4	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	4	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	4	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	4	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	4	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	4	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	4	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	4	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	4	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	5	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	5	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	5	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	5	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	5	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	5	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	5	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	5	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	5	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	5	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	5	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	5	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	5	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	5	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	5	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	5	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	5	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	5	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	5	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	5	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	5	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	5	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	5	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	5	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	5	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	5	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	5	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	5	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	5	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	5	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	6	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	6	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	6	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	6	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	6	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	6	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	6	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	6	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	6	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	6	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	6	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	6	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	6	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	6	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	6	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	6	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	6	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	6	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	6	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	6	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	6	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	6	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	6	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	6	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	6	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	6	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	6	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	6	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	6	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	7	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	7	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	7	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	7	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	7	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	7	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	7	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	7	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	7	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	7	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	7	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	7	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	7	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	7	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	7	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	7	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	7	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	7	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	7	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	7	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	7	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	7	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	7	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	7	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	7	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	7	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	7	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	7	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	7	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	8	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	8	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	8	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	8	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	8	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	8	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	8	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	8	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	8	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	8	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	8	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	8	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	8	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	8	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	8	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	8	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	8	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	8	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	8	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	8	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	8	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	8	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	8	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	8	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	8	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	8	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	8	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	8	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	8	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	8	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	9	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	9	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	9	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	9	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	9	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	9	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	9	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	9	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	9	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	9	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	9	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	9	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	9	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	9	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	9	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	9	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	9	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	9	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	9	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	9	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	9	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	9	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	9	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	9	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	9	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	9	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	9	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	9	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	9	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	10	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	10	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	10	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	10	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	10	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	10	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	10	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	10	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	10	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	10	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	10	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	10	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	10	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	10	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	10	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	10	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	10	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	10	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	10	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	10	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	10	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	10	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	10	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	10	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	10	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	10	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	10	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	10	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	10	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	11	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	11	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	11	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	11	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	11	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	11	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	11	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	11	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	11	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	11	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	11	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	11	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	11	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	11	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	11	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	11	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	11	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	11	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	11	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	11	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	11	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	11	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	11	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	11	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	11	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	11	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	11	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	11	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	11	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	12	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	12	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	12	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	12	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	12	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	12	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	12	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	12	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	12	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	12	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	12	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	12	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	12	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	12	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	12	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	12	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	12	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	12	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	12	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	12	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	12	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	12	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	12	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	12	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	12	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	12	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	12	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	12	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	12	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	12	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	13	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	13	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	13	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	13	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	13	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	13	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	13	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	13	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	13	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	13	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	13	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	13	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	13	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	13	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	13	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	13	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	13	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	13	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	13	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	13	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	13	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	13	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	13	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	13	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	13	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	13	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	13	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	13	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	13	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	14	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	14	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	14	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	14	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	14	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	14	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	14	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	14	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	14	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	14	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	14	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	14	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	14	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	14	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	14	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	14	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	14	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	14	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	14	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	14	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	14	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	14	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	14	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	14	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	14	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	14	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	14	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	14	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	14	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	15	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	15	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	15	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	15	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	15	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	15	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	15	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	15	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	15	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	15	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	15	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	15	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	15	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	15	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	15	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	15	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	15	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	15	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	15	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	15	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	15	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	15	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	15	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	15	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	15	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	15	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	15	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	15	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	15	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	15	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	16	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	16	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	16	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	16	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	16	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	16	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	16	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	16	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	16	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	16	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	16	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	16	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	16	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	16	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	16	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	16	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	16	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	16	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	16	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	16	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	16	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	16	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	16	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	16	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	16	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	16	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	16	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	16	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	16	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	17	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	17	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	17	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	17	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	17	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	17	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	17	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	17	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	17	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	17	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	17	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	17	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	17	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	17	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	17	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	17	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	17	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	17	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	17	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	17	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	17	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	17	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	17	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	17	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	17	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	17	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	17	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	17	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	17	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	17	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	18	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	18	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	18	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	18	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	18	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	18	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	18	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	18	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	18	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	18	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	18	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	18	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	18	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	18	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	18	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	18	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	18	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	18	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	18	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	18	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	18	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	18	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	18	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	18	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	18	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	18	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	18	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	18	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	18	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	19	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	19	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	19	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	19	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	19	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	19	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	19	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	19	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	19	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	19	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	19	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	19	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	19	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	19	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	19	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	19	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	19	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	19	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	19	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	19	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	19	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	19	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	19	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	19	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	19	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	19	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	19	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	19	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	19	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	19	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	20	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	20	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	20	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	20	0.65
(1,751)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	20	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	20	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	20	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	20	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	20	0.65
(1,751)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	20	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	20	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	20	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	20	0.65
(1,751)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	20	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	20	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	20	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	20	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	20	0.65
(1,751)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	20	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	20	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	20	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	20	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	20	0.65
(1,751)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	20	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	20	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	20	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	20	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	20	0.65
(1,751)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	20	0.65
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	8	0.65
(1,587)	1:60:A:ILE:HG21	1:90:A:PHE:HZ	16	0.65
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	16	0.65
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	17	0.65
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	7	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	1	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	1	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	1	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	1	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	1	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	1	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	1	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	1	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	1	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	1	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	1	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	1	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	1	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	1	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	1	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	1	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	1	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	1	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	1	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	1	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	1	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	1	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	1	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	1	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	1	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	1	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	1	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	1	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	1	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	2	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	2	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	2	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	2	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	2	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	2	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	2	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	2	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	2	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	2	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	2	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	2	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	2	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	2	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	2	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	2	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	2	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	2	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	2	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	2	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	2	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	2	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	2	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	2	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	2	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	2	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	2	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	2	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	2	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	3	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	3	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	3	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	3	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	3	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	3	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	3	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	3	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	3	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	3	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	3	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	3	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	3	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	3	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	3	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	3	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	3	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	3	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	3	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	3	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	3	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	3	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	3	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	3	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	3	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	3	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	3	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	3	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	3	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	3	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	4	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	4	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	4	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	4	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	4	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	4	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	4	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	4	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	4	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	4	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	4	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	4	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	4	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	4	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	4	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	4	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	4	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	4	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	4	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	4	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	4	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	4	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	4	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	4	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	4	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	4	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	4	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	4	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	4	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	5	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	5	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	5	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	5	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	5	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	5	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	5	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	5	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	5	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	5	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	5	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	5	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	5	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	5	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	5	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	5	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	5	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	5	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	5	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	5	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	5	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	5	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	5	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	5	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	5	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	5	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	5	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	5	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	5	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	5	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	6	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	6	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	6	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	6	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	6	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	6	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	6	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	6	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	6	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	6	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	6	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	6	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	6	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	6	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	6	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	6	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	6	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	6	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	6	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	6	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	6	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	6	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	6	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	6	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	6	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	6	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	6	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	6	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	6	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	6	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	7	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	7	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	7	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	7	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	7	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	7	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	7	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	7	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	7	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	7	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	7	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	7	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	7	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	7	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	7	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	7	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	7	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	7	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	7	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	7	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	7	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	7	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	7	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	7	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	7	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	7	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	7	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	7	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	7	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	8	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	8	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	8	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	8	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	8	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	8	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	8	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	8	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	8	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	8	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	8	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	8	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	8	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	8	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	8	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	8	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	8	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	8	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	8	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	8	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	8	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	8	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	8	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	8	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	8	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	8	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	8	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	8	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	8	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	9	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	9	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	9	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	9	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	9	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	9	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	9	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	9	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	9	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	9	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	9	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	9	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	9	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	9	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	9	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	9	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	9	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	9	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	9	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	9	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	9	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	9	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	9	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	9	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	9	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	9	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	9	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	9	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	9	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	10	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	10	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	10	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	10	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	10	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	10	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	10	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	10	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	10	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	10	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	10	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	10	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	10	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	10	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	10	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	10	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	10	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	10	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	10	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	10	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	10	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	10	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	10	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	10	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	10	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	10	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	10	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	10	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	10	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	10	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	11	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	11	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	11	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	11	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	11	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	11	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	11	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	11	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	11	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	11	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	11	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	11	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	11	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	11	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	11	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	11	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	11	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	11	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	11	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	11	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	11	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	11	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	11	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	11	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	11	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	11	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	11	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	11	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	11	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	11	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	12	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	12	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	12	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	12	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	12	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	12	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	12	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	12	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	12	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	12	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	12	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	12	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	12	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	12	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	12	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	12	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	12	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	12	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	12	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	12	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	12	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	12	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	12	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	12	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	12	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	12	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	12	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	12	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	12	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	12	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	13	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	13	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	13	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	13	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	13	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	13	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	13	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	13	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	13	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	13	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	13	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	13	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	13	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	13	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	13	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	13	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	13	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	13	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	13	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	13	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	13	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	13	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	13	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	13	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	13	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	13	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	13	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	13	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	13	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	13	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	14	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	14	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	14	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	14	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	14	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	14	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	14	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	14	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	14	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	14	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	14	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	14	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	14	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	14	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	14	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	14	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	14	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	14	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	14	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	14	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	14	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	14	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	14	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	14	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	14	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	14	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	14	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	14	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	14	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	15	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	15	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	15	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	15	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	15	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	15	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	15	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	15	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	15	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	15	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	15	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	15	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	15	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	15	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	15	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	15	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	15	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	15	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	15	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	15	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	15	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	15	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	15	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	15	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	15	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	15	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	15	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	15	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	15	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	16	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	16	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	16	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	16	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	16	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	16	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	16	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	16	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	16	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	16	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	16	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	16	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	16	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	16	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	16	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	16	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	16	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	16	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	16	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	16	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	16	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	16	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	16	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	16	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	16	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	16	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	16	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	16	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	16	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	17	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	17	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	17	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	17	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	17	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	17	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	17	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	17	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	17	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	17	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	17	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	17	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	17	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	17	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	17	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	17	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	17	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	17	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	17	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	17	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	17	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	17	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	17	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	17	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	17	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	17	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	17	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	17	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	17	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	17	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	18	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	18	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	18	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	18	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	18	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	18	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	18	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	18	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	18	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	18	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	18	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	18	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	18	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	18	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	18	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	18	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	18	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	18	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	18	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	18	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	18	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	18	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	18	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	18	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	18	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	18	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	18	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	18	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	18	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	19	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	19	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	19	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	19	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	19	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	19	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	19	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	19	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	19	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	19	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	19	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	19	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	19	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	19	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	19	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	19	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	19	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	19	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	19	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	19	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	19	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	19	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	19	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	19	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	19	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	19	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	19	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	19	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	19	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	19	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD12	20	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD13	20	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD21	20	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD22	20	0.65
(1,26)	1:6:A:LEU:HD11	1:6:A:LEU:HD23	20	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD11	20	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD13	20	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD21	20	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD22	20	0.65
(1,26)	1:6:A:LEU:HD12	1:6:A:LEU:HD23	20	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD11	20	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD12	20	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD21	20	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD22	20	0.65
(1,26)	1:6:A:LEU:HD13	1:6:A:LEU:HD23	20	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD11	20	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD12	20	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD13	20	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD22	20	0.65
(1,26)	1:6:A:LEU:HD21	1:6:A:LEU:HD23	20	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD11	20	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD12	20	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD13	20	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD21	20	0.65
(1,26)	1:6:A:LEU:HD22	1:6:A:LEU:HD23	20	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD11	20	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD12	20	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD13	20	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD21	20	0.65
(1,26)	1:6:A:LEU:HD23	1:6:A:LEU:HD22	20	0.65
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD12	19	0.64
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD13	19	0.64
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD21	19	0.64
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD22	19	0.64
(1,2732)	1:101:B:LEU:HD11	1:101:B:LEU:HD23	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD11	19	0.64
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD13	19	0.64
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD21	19	0.64
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD22	19	0.64
(1,2732)	1:101:B:LEU:HD12	1:101:B:LEU:HD23	19	0.64
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD11	19	0.64
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD12	19	0.64
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD21	19	0.64
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD22	19	0.64
(1,2732)	1:101:B:LEU:HD13	1:101:B:LEU:HD23	19	0.64
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD11	19	0.64
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD12	19	0.64
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD13	19	0.64
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD22	19	0.64
(1,2732)	1:101:B:LEU:HD21	1:101:B:LEU:HD23	19	0.64
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD11	19	0.64
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD12	19	0.64
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD13	19	0.64
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD21	19	0.64
(1,2732)	1:101:B:LEU:HD22	1:101:B:LEU:HD23	19	0.64
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD11	19	0.64
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD12	19	0.64
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD13	19	0.64
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD21	19	0.64
(1,2732)	1:101:B:LEU:HD23	1:101:B:LEU:HD22	19	0.64
(1,2697)	1:69:B:THR:HG21	1:98:B:ILE:HA	14	0.64
(1,2465)	1:68:B:LEU:HD12	1:66:B:ILE:HG12	8	0.64
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	8	0.64
(1,1959)	1:89:B:THR:HG23	1:87:B:LEU:HB2	12	0.64
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	6	0.64
(1,1745)	1:43:B:ILE:HG21	1:65:B:PHE:HB3	17	0.64
(1,1725)	1:64:B:ASP:HB2	1:43:B:ILE:HG22	2	0.64
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	2	0.64
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	12	0.64
(1,1380)	1:103:A:THR:HG22	1:105:A:ILE:HB	20	0.64
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	12	0.64
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	18	0.64
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	20	0.64
(1,1959)	1:89:B:THR:HG21	1:87:B:LEU:HB2	17	0.63
(1,1959)	1:89:B:THR:HG21	1:87:B:LEU:HB2	20	0.63
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	13	0.63
(1,1403)	1:6:B:LEU:HB2	1:5:B:THR:HG21	11	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	13	0.63
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	5	0.63
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	15	0.63
(1,1081)	1:68:A:LEU:HD11	1:66:A:ILE:HG12	14	0.63
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	9	0.63
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG21	14	0.63
(1,643)	1:94:A:ILE:HG21	1:24:A:VAL:HG22	12	0.63
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG23	18	0.63
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG22	19	0.63
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	18	0.63
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD13	16	0.63
(1,341)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	16	0.63
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	3	0.63
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	18	0.63
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG22	3	0.63
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	4	0.62
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	17	0.62
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD13	5	0.62
(1,1722)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	5	0.62
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	8	0.62
(1,1403)	1:6:B:LEU:HB2	1:5:B:THR:HG21	16	0.62
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	1	0.62
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG21	3	0.62
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	15	0.62
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG21	1	0.62
(1,2758)	1:103:B:THR:HG21	1:102:B:ILE:HG23	14	0.61
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	12	0.61
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	17	0.61
(1,1959)	1:89:B:THR:HG23	1:87:B:LEU:HB2	8	0.61
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	9	0.61
(1,1853)	1:11:B:ASP:HB3	1:79:B:ILE:HG13	12	0.61
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	13	0.61
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG23	14	0.61
(1,1313)	1:69:A:THR:HG22	1:98:A:ILE:HA	4	0.61
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	12	0.61
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	11	0.61
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG21	2	0.61
(1,661)	1:97:A:ALA:HA	1:69:A:THR:HG1	19	0.61
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	3	0.61
(1,341)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	10	0.61
(1,2697)	1:69:B:THR:HG21	1:98:B:ILE:HA	6	0.6
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	14	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG23	16	0.6
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	19	0.6
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	17	0.6
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD13	8	0.6
(1,1722)	1:64:B:ASP:HB2	1:43:B:ILE:HG22	2	0.6
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	4	0.6
(1,1313)	1:69:A:THR:HG21	1:98:A:ILE:HA	9	0.6
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG1	12	0.6
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	13	0.6
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG22	6	0.6
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	8	0.6
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	11	0.6
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG22	16	0.6
(1,2672)	1:94:B:ILE:HG13	1:90:B:PHE:HB3	6	0.59
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	1	0.59
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	2	0.59
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG23	12	0.59
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG23	16	0.59
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG21	2	0.59
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	6	0.59
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	1	0.59
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	19	0.59
(1,575)	1:89:A:THR:HG22	1:87:A:LEU:HB2	3	0.59
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	17	0.59
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	4	0.59
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	9	0.59
(1,338)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	16	0.59
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	3	0.59
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	13	0.59
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	18	0.58
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG22	16	0.58
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG23	14	0.58
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	10	0.58
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	4	0.58
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	5	0.58
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	19	0.58
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG23	20	0.58
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	9	0.58
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG22	10	0.58
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	2	0.58
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	20	0.58
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	2	0.58
(1,498)	1:80:A:LEU:HA	1:79:A:ILE:HG13	7	0.58
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	11	0.58
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	16	0.58
(1,3069)	1:66:B:ILE:H	1:43:B:ILE:HG22	17	0.57
(1,2697)	1:69:B:THR:HG22	1:98:B:ILE:HA	15	0.57
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG21	10	0.57
(1,2053)	1:69:B:THR:HG21	1:98:B:ILE:H	20	0.57
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	11	0.57
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	4	0.57
(1,1726)	1:57:B:THR:HG23	1:64:B:ASP:HB3	20	0.57
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	3	0.57
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	5	0.57
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	10	0.57
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	7	0.57
(1,587)	1:60:A:ILE:HG13	1:90:A:PHE:HZ	15	0.57
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	10	0.57
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	11	0.57
(1,338)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	10	0.57
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	10	0.56
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG21	1	0.56
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG21	5	0.56
(1,2073)	1:69:B:THR:HG1	1:100:B:PHE:HD2	4	0.56
(1,2053)	1:69:B:THR:HG21	1:98:B:ILE:H	17	0.56
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	6	0.56
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	9	0.56
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	7	0.56
(1,1288)	1:94:A:ILE:HG12	1:90:A:PHE:HB2	7	0.56
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	4	0.56
(1,564)	1:87:A:LEU:HD23	1:60:A:ILE:HG23	7	0.56
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	20	0.56
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	16	0.56
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	12	0.56
(1,416)	1:37:A:VAL:HG23	1:73:A:THR:HG21	1	0.56
(1,409)	1:69:A:THR:HG23	1:54:A:LEU:HA	2	0.56
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	3	0.56
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	13	0.56
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	9	0.56
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	2	0.56
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	16	0.55
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG22	11	0.55
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1971)	1:60:B:ILE:HG21	1:90:B:PHE:HZ	9	0.55
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	18	0.55
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG22	16	0.55
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	3	0.55
(1,1313)	1:69:A:THR:HG21	1:98:A:ILE:HA	11	0.55
(1,1313)	1:69:A:THR:HG21	1:98:A:ILE:HA	17	0.55
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG21	8	0.55
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG21	8	0.55
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	8	0.55
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD12	1	0.55
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	14	0.55
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	4	0.55
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG21	5	0.55
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG23	2	0.55
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	1	0.54
(1,2697)	1:69:B:THR:HG23	1:98:B:ILE:HA	7	0.54
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	9	0.54
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG21	2	0.54
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	5	0.54
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	11	0.54
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	19	0.54
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	1	0.54
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	4	0.54
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG23	11	0.54
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG23	7	0.54
(1,1356)	1:102:A:ILE:HG13	1:101:A:LEU:HG	19	0.54
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG22	3	0.54
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	17	0.54
(1,327)	1:60:A:ILE:HG13	1:58:A:ILE:HD12	15	0.54
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	8	0.54
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	17	0.54
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	20	0.54
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	5	0.53
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG23	4	0.53
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	3	0.53
(1,1793)	1:69:B:THR:HG22	1:54:B:LEU:HA	12	0.53
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD13	9	0.53
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	6	0.53
(1,1403)	1:6:B:LEU:HB2	1:5:B:THR:HG21	8	0.53
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG13	18	0.53
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	16	0.53
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	18	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG22	11	0.53
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG22	10	0.53
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD2	13	0.53
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	5	0.53
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	19	0.53
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG21	16	0.53
(1,19)	1:6:A:LEU:HB2	1:5:A:THR:HG23	18	0.53
(1,2671)	1:90:B:PHE:HB3	1:94:B:ILE:HG13	6	0.52
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	3	0.52
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	19	0.52
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG23	5	0.52
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	9	0.52
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	8	0.52
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	19	0.52
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	17	0.52
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	4	0.52
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	13	0.52
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG23	1	0.52
(1,421)	1:71:A:GLN:HB2	1:73:A:THR:HG21	18	0.52
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD11	15	0.52
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	4	0.52
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	8	0.52
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	12	0.52
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	1	0.52
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG21	9	0.52
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	5	0.51
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	2	0.51
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	6	0.51
(1,1948)	1:87:B:LEU:HD13	1:60:B:ILE:HG23	2	0.51
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG22	12	0.51
(1,1751)	1:58:B:ILE:HG13	1:65:B:PHE:HD2	15	0.51
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	13	0.51
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	5	0.51
(1,1571)	1:34:B:THR:HG22	1:34:B:THR:HA	13	0.51
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	10	0.51
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	11	0.51
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	15	0.51
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	18	0.51
(1,564)	1:87:A:LEU:HD13	1:60:A:ILE:HG23	1	0.51
(1,564)	1:87:A:LEU:HD12	1:60:A:ILE:HG23	12	0.51
(1,564)	1:87:A:LEU:HD12	1:60:A:ILE:HG23	13	0.51
(1,544)	1:85:A:ASN:HB2	1:60:A:ILE:HG23	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	9	0.51
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	2	0.51
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	13	0.51
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	15	0.51
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	12	0.51
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	1	0.5
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	10	0.5
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	20	0.5
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG21	18	0.5
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG22	20	0.5
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG23	1	0.5
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG23	19	0.5
(1,1313)	1:69:A:THR:HG21	1:98:A:ILE:HA	10	0.5
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	14	0.5
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	1	0.5
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB3	4	0.5
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG21	13	0.5
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	1	0.5
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	7	0.5
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	10	0.5
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	14	0.5
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD11	4	0.5
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	19	0.5
(1,321)	1:59:A:HIS:HB2	1:57:A:THR:HG1	7	0.5
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	1	0.5
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	11	0.5
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	12	0.5
(1,2376)	1:58:B:ILE:HG12	1:56:B:PRO:HB2	17	0.49
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	20	0.49
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG23	14	0.49
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	18	0.49
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	14	0.49
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD13	1	0.49
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	10	0.49
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	6	0.49
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	2	0.49
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG22	18	0.49
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG21	16	0.49
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG23	14	0.49
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG22	15	0.49
(1,669)	1:69:A:THR:HG22	1:98:A:ILE:H	4	0.49
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	13	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	17	0.49
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	20	0.49
(1,575)	1:89:A:THR:HG1	1:87:A:LEU:HB2	8	0.49
(1,544)	1:85:A:ASN:HB2	1:60:A:ILE:HG23	16	0.49
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	9	0.49
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	20	0.49
(1,342)	1:57:A:THR:HG21	1:64:A:ASP:HB3	18	0.49
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD13	11	0.49
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	11	0.49
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	10	0.49
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	14	0.49
(1,2673)	1:94:B:ILE:HG13	1:90:B:PHE:HB3	2	0.48
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG13	4	0.48
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	9	0.48
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	9	0.48
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	7	0.48
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	13	0.48
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	14	0.48
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	16	0.48
(1,1959)	1:89:B:THR:HG1	1:87:B:LEU:HB2	11	0.48
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	11	0.48
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG22	1	0.48
(1,1805)	1:71:B:GLN:HB2	1:73:B:THR:HG23	12	0.48
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD12	7	0.48
(1,1754)	1:60:B:ILE:HG22	1:65:B:PHE:HD2	15	0.48
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD2	2	0.48
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	8	0.48
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	10	0.48
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	18	0.48
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD12	10	0.48
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	10	0.48
(1,1287)	1:90:A:PHE:HB2	1:94:A:ILE:HG12	7	0.48
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	6	0.48
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	12	0.48
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	13	0.48
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG23	12	0.48
(1,410)	1:69:A:THR:HG22	1:56:A:PRO:HD3	2	0.48
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	15	0.48
(1,336)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	11	0.48
(1,312)	1:58:A:ILE:HG13	1:57:A:THR:HB	5	0.48
(1,311)	1:58:A:ILE:HG13	1:57:A:THR:HB	5	0.48
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	15	0.48
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	4	0.47
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB3	19	0.47
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	4	0.47
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	5	0.47
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	19	0.47
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	4	0.47
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG13	7	0.47
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG23	17	0.47
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG12	17	0.47
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	10	0.47
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	7	0.47
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	9	0.47
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	18	0.47
(1,1313)	1:69:A:THR:HG22	1:98:A:ILE:HA	1	0.47
(1,701)	1:69:A:THR:HG22	1:101:A:LEU:HB3	13	0.47
(1,701)	1:69:A:THR:HG23	1:101:A:LEU:HB3	14	0.47
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	11	0.47
(1,669)	1:69:A:THR:HG23	1:98:A:ILE:H	5	0.47
(1,669)	1:69:A:THR:HG21	1:98:A:ILE:H	9	0.47
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	4	0.47
(1,564)	1:87:A:LEU:HD13	1:60:A:ILE:HG23	6	0.47
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	19	0.47
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	13	0.47
(1,416)	1:37:A:VAL:HG22	1:73:A:THR:HG1	5	0.47
(1,416)	1:37:A:VAL:HG23	1:73:A:THR:HG21	19	0.47
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	2	0.47
(1,327)	1:60:A:ILE:HG21	1:58:A:ILE:HD13	1	0.47
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG1	8	0.47
(1,266)	1:44:A:GLU:HB2	1:43:A:ILE:HG21	16	0.47
(1,187)	1:34:A:THR:HG23	1:34:A:THR:HA	19	0.47
(1,2500)	1:75:B:VAL:HG13	1:73:B:THR:HG1	13	0.46
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	9	0.46
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG23	15	0.46
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB2	16	0.46
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	8	0.46
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	18	0.46
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG23	15	0.46
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG23	8	0.46
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	6	0.46
(1,1313)	1:69:A:THR:HG21	1:98:A:ILE:HA	19	0.46
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG21	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB2	9	0.46
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	14	0.46
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	8	0.46
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	5	0.46
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD12	6	0.46
(1,311)	1:58:A:ILE:HG13	1:57:A:THR:HB	19	0.46
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG21	12	0.46
(1,187)	1:34:A:THR:HG21	1:34:A:THR:HA	5	0.46
(1,187)	1:34:A:THR:HG21	1:34:A:THR:HA	8	0.46
(1,2574)	1:5:B:THR:HG21	1:83:B:PRO:HG3	15	0.45
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	15	0.45
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG21	19	0.45
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	13	0.45
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	18	0.45
(1,1959)	1:89:B:THR:HG1	1:87:B:LEU:HB2	14	0.45
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG22	8	0.45
(1,1695)	1:58:B:ILE:HG13	1:57:B:THR:HB	1	0.45
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	4	0.45
(1,1571)	1:34:B:THR:HG22	1:34:B:THR:HA	10	0.45
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	5	0.45
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG21	4	0.45
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG21	11	0.45
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	17	0.45
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	20	0.45
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG23	10	0.45
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	17	0.45
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	10	0.45
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	2	0.45
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	10	0.45
(1,336)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	7	0.45
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	5	0.44
(1,2574)	1:5:B:THR:HG21	1:83:B:PRO:HG3	17	0.44
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	7	0.44
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	12	0.44
(1,1971)	1:60:B:ILE:HG22	1:90:B:PHE:HZ	1	0.44
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG21	8	0.44
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	16	0.44
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	19	0.44
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	6	0.44
(1,1794)	1:69:B:THR:HG1	1:56:B:PRO:HD3	18	0.44
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	1	0.44
(1,1376)	1:103:A:THR:HG1	1:103:A:THR:HA	20	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:69:A:THR:HG1	1:98:A:ILE:HA	16	0.44
(1,1285)	1:94:A:ILE:HG21	1:4:A:PHE:HD1	10	0.44
(1,1190)	1:5:A:THR:HG22	1:83:A:PRO:HG3	5	0.44
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	12	0.44
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	7	0.44
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG12	4	0.44
(1,701)	1:69:A:THR:HG23	1:101:A:LEU:HB3	18	0.44
(1,669)	1:69:A:THR:HG21	1:98:A:ILE:H	7	0.44
(1,669)	1:69:A:THR:HG21	1:98:A:ILE:H	17	0.44
(1,669)	1:69:A:THR:HG21	1:98:A:ILE:H	19	0.44
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	9	0.44
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG21	6	0.44
(1,416)	1:37:A:VAL:HG22	1:73:A:THR:HG23	18	0.44
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	3	0.44
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD12	3	0.44
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	11	0.44
(1,336)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	18	0.44
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG1	14	0.44
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	7	0.44
(1,3061)	1:60:B:ILE:H	1:58:B:ILE:HG13	1	0.43
(1,2376)	1:58:B:ILE:HG13	1:56:B:PRO:HB2	4	0.43
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG1	13	0.43
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	19	0.43
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG12	19	0.43
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	20	0.43
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	13	0.43
(1,1804)	1:73:B:THR:HG21	1:39:B:PRO:HG3	4	0.43
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	7	0.43
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	8	0.43
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG21	17	0.43
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	4	0.43
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG23	6	0.43
(1,1403)	1:6:B:LEU:HB2	1:5:B:THR:HG23	17	0.43
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	18	0.43
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	20	0.43
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	15	0.43
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG21	5	0.43
(1,669)	1:69:A:THR:HG1	1:98:A:ILE:H	16	0.43
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	2	0.43
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	3	0.43
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	20	0.43
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG22	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD12	11	0.43
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	5	0.43
(1,187)	1:34:A:THR:HG21	1:34:A:THR:HA	7	0.43
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB2	8	0.42
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG13	12	0.42
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	3	0.42
(1,1991)	1:91:B:ARG:HD3	1:89:B:THR:HG1	17	0.42
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	8	0.42
(1,1794)	1:69:B:THR:HG1	1:56:B:PRO:HD3	9	0.42
(1,1724)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	2	0.42
(1,1711)	1:60:B:ILE:HG21	1:58:B:ILE:HD13	2	0.42
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	5	0.42
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	19	0.42
(1,1190)	1:5:A:THR:HG23	1:83:A:PRO:HG3	6	0.42
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	15	0.42
(1,723)	1:98:A:ILE:HD11	1:102:A:ILE:HG13	12	0.42
(1,587)	1:60:A:ILE:HG22	1:90:A:PHE:HZ	19	0.42
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	17	0.42
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	20	0.42
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	12	0.42
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	17	0.42
(1,309)	1:57:A:THR:HG23	1:58:A:ILE:HA	16	0.42
(1,309)	1:57:A:THR:HG21	1:58:A:ILE:HA	19	0.42
(1,302)	1:57:A:THR:HG21	1:43:A:ILE:HB	18	0.42
(1,187)	1:34:A:THR:HG23	1:34:A:THR:HA	6	0.42
(1,187)	1:34:A:THR:HG22	1:34:A:THR:HA	10	0.42
(1,2803)	1:60:A:ILE:H	1:58:A:ILE:HG13	10	0.41
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG22	6	0.41
(1,2697)	1:69:B:THR:HG21	1:98:B:ILE:HA	4	0.41
(1,2574)	1:5:B:THR:HG23	1:83:B:PRO:HG3	2	0.41
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB2	6	0.41
(1,2114)	1:103:B:THR:HG22	1:99:B:ASP:HB2	9	0.41
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB2	20	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	1	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	1	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	3	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	3	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	4	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	4	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	5	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	5	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	6	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	7	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	7	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	10	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	10	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	11	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	11	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	12	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	12	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	14	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	14	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	15	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	15	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	16	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	16	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	17	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	17	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	18	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	18	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	19	0.41
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	19	0.41
(1,1882)	1:80:B:LEU:HA	1:79:B:ILE:HG13	20	0.41
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	17	0.41
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	17	0.41
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	17	0.41
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	3	0.41
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	15	0.41
(1,1800)	1:37:B:VAL:HG23	1:73:B:THR:HG1	20	0.41
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	11	0.41
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	20	0.41
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD12	4	0.41
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	1	0.41
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	19	0.41
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG13	4	0.41
(1,1048)	1:41:A:THR:HG22	1:66:A:ILE:HB	5	0.41
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	7	0.41
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG21	3	0.41
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	6	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	2	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	2	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	3	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	6	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	6	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	8	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	8	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	9	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	9	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	10	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	10	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	11	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	11	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	12	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	12	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	13	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	13	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	14	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	14	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	16	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	16	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	18	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	18	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	19	0.41
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	19	0.41
(1,607)	1:91:A:ARG:HD3	1:89:A:THR:HG1	14	0.41
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	6	0.41
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	13	0.41
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	17	0.41
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	11	0.41
(1,409)	1:69:A:THR:HG23	1:54:A:LEU:HA	16	0.41
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	7	0.41
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD2	1	0.41
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	12	0.41
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	13	0.41
(1,187)	1:34:A:THR:HG22	1:34:A:THR:HA	1	0.41
(1,2574)	1:5:B:THR:HG21	1:83:B:PRO:HG3	6	0.4
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	16	0.4
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	2	0.4
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG21	2	0.4
(1,2107)	1:98:B:ILE:HD13	1:102:B:ILE:HG21	17	0.4
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG13	18	0.4
(1,2085)	1:69:B:THR:HG21	1:101:B:LEU:HB3	4	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	2	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	8	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	8	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	9	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	9	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	13	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	13	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG2	20	0.4
(1,1999)	1:91:B:ARG:HA	1:91:B:ARG:HG3	20	0.4
(1,1948)	1:87:B:LEU:HD21	1:60:B:ILE:HG23	10	0.4
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	7	0.4
(1,1859)	1:79:B:ILE:HG21	1:78:B:LYS:HG2	1	0.4
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	13	0.4
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	18	0.4
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	4	0.4
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	12	0.4
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	14	0.4
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	2	0.4
(1,1720)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	5	0.4
(1,1696)	1:58:B:ILE:HG13	1:57:B:THR:HB	4	0.4
(1,1695)	1:58:B:ILE:HG13	1:57:B:THR:HB	4	0.4
(1,1693)	1:57:B:THR:HG21	1:58:B:ILE:HA	4	0.4
(1,1571)	1:34:B:THR:HG21	1:34:B:THR:HA	15	0.4
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG23	3	0.4
(1,1374)	1:103:A:THR:HG23	1:102:A:ILE:HG23	5	0.4
(1,1289)	1:94:A:ILE:HG12	1:90:A:PHE:HB3	1	0.4
(1,1190)	1:5:A:THR:HG22	1:83:A:PRO:HG3	1	0.4
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG21	12	0.4
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB2	8	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	1	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	1	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	4	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	4	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	5	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	5	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	7	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	7	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	15	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	15	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	17	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	17	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG2	20	0.4
(1,615)	1:91:A:ARG:HA	1:91:A:ARG:HG3	20	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG21	10	0.4
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	16	0.4
(1,417)	1:37:A:VAL:HG23	1:73:A:THR:HG21	1	0.4
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	5	0.4
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	15	0.4
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	19	0.4
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD12	12	0.4
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD13	17	0.4
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD13	19	0.4
(1,309)	1:57:A:THR:HG23	1:58:A:ILE:HA	1	0.4
(1,309)	1:57:A:THR:HG21	1:58:A:ILE:HA	3	0.4
(1,309)	1:57:A:THR:HG21	1:58:A:ILE:HA	15	0.4
(1,309)	1:57:A:THR:HG21	1:58:A:ILE:HA	20	0.4
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	15	0.4
(1,2758)	1:103:B:THR:HG21	1:102:B:ILE:HG22	9	0.39
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	4	0.39
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	9	0.39
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	6	0.39
(1,2121)	1:105:B:ILE:HG21	1:99:B:ASP:HA	19	0.39
(1,2114)	1:103:B:THR:HG21	1:99:B:ASP:HB2	3	0.39
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG13	7	0.39
(1,2073)	1:69:B:THR:HG1	1:100:B:PHE:HD2	7	0.39
(1,1948)	1:87:B:LEU:HD13	1:60:B:ILE:HG21	5	0.39
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	5	0.39
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	19	0.39
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	19	0.39
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG21	6	0.39
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	18	0.39
(1,1716)	1:61:B:ASP:HB3	1:60:B:ILE:HG13	12	0.39
(1,1693)	1:57:B:THR:HG22	1:58:B:ILE:HA	9	0.39
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	5	0.39
(1,1571)	1:34:B:THR:HG23	1:34:B:THR:HA	16	0.39
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	7	0.39
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	7	0.39
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	4	0.39
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	4	0.39
(1,1289)	1:94:A:ILE:HG13	1:90:A:PHE:HB3	18	0.39
(1,1190)	1:5:A:THR:HG22	1:83:A:PRO:HG3	14	0.39
(1,1048)	1:41:A:THR:HG22	1:66:A:ILE:HB	2	0.39
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG23	15	0.39
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	10	0.39
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	11	0.39
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	11	0.39
(1,730)	1:103:A:THR:HG21	1:99:A:ASP:HB2	5	0.39
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG13	20	0.39
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	19	0.39
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG21	5	0.39
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	19	0.39
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	4	0.39
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG1	15	0.39
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	18	0.39
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD12	18	0.39
(1,309)	1:57:A:THR:HG22	1:58:A:ILE:HA	10	0.39
(1,309)	1:57:A:THR:HG22	1:58:A:ILE:HA	11	0.39
(1,309)	1:57:A:THR:HG23	1:58:A:ILE:HA	13	0.39
(1,309)	1:57:A:THR:HG1	1:58:A:ILE:HA	18	0.39
(1,187)	1:34:A:THR:HG21	1:34:A:THR:HA	2	0.39
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	19	0.38
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	19	0.38
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	2	0.38
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	2	0.38
(1,2672)	1:94:B:ILE:HG13	1:90:B:PHE:HB3	2	0.38
(1,2574)	1:5:B:THR:HG21	1:83:B:PRO:HG3	14	0.38
(1,2432)	1:41:B:THR:HG21	1:66:B:ILE:HB	6	0.38
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	4	0.38
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	4	0.38
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	9	0.38
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG13	14	0.38
(1,2107)	1:98:B:ILE:HD13	1:102:B:ILE:HG13	20	0.38
(1,2027)	1:94:B:ILE:HG21	1:24:B:VAL:HG12	9	0.38
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	18	0.38
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	3	0.38
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG21	9	0.38
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG21	3	0.38
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG21	9	0.38
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	13	0.38
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	6	0.38
(1,1725)	1:64:B:ASP:HB2	1:43:B:ILE:HG13	1	0.38
(1,1693)	1:57:B:THR:HG1	1:58:B:ILE:HA	3	0.38
(1,1693)	1:57:B:THR:HG21	1:58:B:ILE:HA	10	0.38
(1,1693)	1:57:B:THR:HG22	1:58:B:ILE:HA	13	0.38
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	15	0.38
(1,1693)	1:57:B:THR:HG22	1:58:B:ILE:HA	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG1	13	0.38
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	7	0.38
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	7	0.38
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	16	0.38
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	16	0.38
(1,1313)	1:69:A:THR:HG23	1:98:A:ILE:HA	18	0.38
(1,1190)	1:5:A:THR:HG22	1:83:A:PRO:HG3	9	0.38
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	19	0.38
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	4	0.38
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	4	0.38
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	12	0.38
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	12	0.38
(1,737)	1:105:A:ILE:HG12	1:99:A:ASP:HA	14	0.38
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG12	15	0.38
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	17	0.38
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	1	0.38
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	2	0.38
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	15	0.38
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	20	0.38
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	9	0.38
(1,416)	1:37:A:VAL:HG23	1:73:A:THR:HG21	4	0.38
(1,416)	1:37:A:VAL:HG22	1:73:A:THR:HG1	16	0.38
(1,309)	1:57:A:THR:HG1	1:58:A:ILE:HA	7	0.38
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	2	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	8	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	8	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	14	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	14	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	18	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	18	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	20	0.38
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	20	0.38
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	17	0.38
(1,2697)	1:69:B:THR:HG1	1:98:B:ILE:HA	12	0.37
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	1	0.37
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	2	0.37
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	2	0.37
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	9	0.37
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	9	0.37
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	12	0.37
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	12	0.37
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	17	0.37
(1,2107)	1:98:B:ILE:HD13	1:102:B:ILE:HG13	3	0.37
(1,2073)	1:69:B:THR:HG1	1:100:B:PHE:HD2	1	0.37
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG23	6	0.37
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	10	0.37
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	16	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	2	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	2	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	3	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	3	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	10	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	10	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	15	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	15	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	17	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	17	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	18	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	18	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	20	0.37
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	20	0.37
(1,1190)	1:5:A:THR:HG22	1:83:A:PRO:HG3	4	0.37
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	8	0.37
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	10	0.37
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	17	0.37
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	19	0.37
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	15	0.37
(1,943)	1:41:A:THR:HG1	1:17:A:THR:HG22	13	0.37
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	9	0.37
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	9	0.37
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	1	0.37
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG13	5	0.37
(1,575)	1:89:A:THR:HG1	1:87:A:LEU:HB2	19	0.37
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	8	0.37
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	8	0.37
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	8	0.37
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	18	0.37
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	18	0.37
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	18	0.37
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	2	0.37
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	3	0.37
(1,475)	1:79:A:ILE:HG21	1:78:A:LYS:HG2	5	0.37
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG22	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	8	0.37
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG22	10	0.37
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	11	0.37
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	18	0.37
(1,336)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	16	0.37
(1,309)	1:57:A:THR:HG23	1:58:A:ILE:HA	2	0.37
(1,309)	1:57:A:THR:HG23	1:58:A:ILE:HA	12	0.37
(1,187)	1:34:A:THR:HG23	1:34:A:THR:HA	12	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	2	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	2	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	3	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	3	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	4	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	4	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	6	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	6	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	17	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	17	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	19	0.37
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	19	0.37
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	13	0.36
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	5	0.36
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	5	0.36
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG23	18	0.36
(1,2114)	1:103:B:THR:HG21	1:99:B:ASP:HB3	6	0.36
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG21	2	0.36
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	8	0.36
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG13	8	0.36
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	12	0.36
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	12	0.36
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	12	0.36
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	11	0.36
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	14	0.36
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG23	16	0.36
(1,1805)	1:71:B:GLN:HB2	1:73:B:THR:HG22	7	0.36
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG23	8	0.36
(1,1794)	1:69:B:THR:HG22	1:56:B:PRO:HD3	8	0.36
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	10	0.36
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	13	0.36
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD12	2	0.36
(1,1693)	1:57:B:THR:HG22	1:58:B:ILE:HA	12	0.36
(1,1686)	1:57:B:THR:HG21	1:43:B:ILE:HB	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1571)	1:34:B:THR:HG23	1:34:B:THR:HA	14	0.36
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	5	0.36
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	5	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	1	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	1	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	5	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	5	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	11	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	11	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	13	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	13	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	19	0.36
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	19	0.36
(1,1422)	1:8:B:LYS:HD2	1:8:B:LYS:HA	11	0.36
(1,1422)	1:8:B:LYS:HD3	1:8:B:LYS:HA	11	0.36
(1,1285)	1:94:A:ILE:HG21	1:4:A:PHE:HD1	16	0.36
(1,1081)	1:68:A:LEU:HD13	1:66:A:ILE:HG12	18	0.36
(1,732)	1:103:A:THR:HB	1:102:A:ILE:HG23	8	0.36
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	7	0.36
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG21	17	0.36
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD21	7	0.36
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	9	0.36
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	9	0.36
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	9	0.36
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	7	0.36
(1,475)	1:79:A:ILE:HG21	1:78:A:LYS:HG2	12	0.36
(1,475)	1:79:A:ILE:HG13	1:78:A:LYS:HG2	15	0.36
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	3	0.36
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG13	5	0.36
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	6	0.36
(1,410)	1:69:A:THR:HG23	1:56:A:PRO:HD3	16	0.36
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	14	0.36
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	3	0.36
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	9	0.36
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	1	0.36
(1,309)	1:57:A:THR:HG23	1:58:A:ILE:HA	4	0.36
(1,302)	1:57:A:THR:HG23	1:43:A:ILE:HB	7	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	7	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	7	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	9	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	9	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	10	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	10	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	11	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	11	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	16	0.36
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	16	0.36
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	14	0.35
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	14	0.35
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	16	0.35
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	16	0.35
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	19	0.35
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	1	0.35
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	1	0.35
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG21	15	0.35
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	16	0.35
(1,2107)	1:98:B:ILE:HD13	1:102:B:ILE:HG13	9	0.35
(1,2107)	1:98:B:ILE:HD13	1:102:B:ILE:HG21	15	0.35
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG13	16	0.35
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	9	0.35
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	9	0.35
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	9	0.35
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	10	0.35
(1,1859)	1:79:B:ILE:HG13	1:78:B:LYS:HG2	20	0.35
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	14	0.35
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	16	0.35
(1,1793)	1:69:B:THR:HG1	1:54:B:LEU:HA	3	0.35
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	19	0.35
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	2	0.35
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	15	0.35
(1,1686)	1:57:B:THR:HG23	1:43:B:ILE:HB	20	0.35
(1,1571)	1:34:B:THR:HG21	1:34:B:THR:HA	9	0.35
(1,1571)	1:34:B:THR:HG22	1:34:B:THR:HA	11	0.35
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	10	0.35
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	10	0.35
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	12	0.35
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	12	0.35
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	6	0.35
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	6	0.35
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	7	0.35
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	12	0.35
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	8	0.35
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	8	0.35
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	9	0.35
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG21	17	0.35
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG13	7	0.35
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG13	9	0.35
(1,689)	1:69:A:THR:HG21	1:100:A:PHE:HD2	10	0.35
(1,669)	1:69:A:THR:HG21	1:98:A:ILE:H	12	0.35
(1,581)	1:58:A:ILE:HG22	1:90:A:PHE:HD2	6	0.35
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	1	0.35
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	1	0.35
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	1	0.35
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	7	0.35
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	12	0.35
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG21	9	0.35
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	4	0.35
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD12	7	0.35
(1,336)	1:43:A:ILE:HG13	1:64:A:ASP:HB2	10	0.35
(1,309)	1:57:A:THR:HG22	1:58:A:ILE:HA	14	0.35
(1,309)	1:57:A:THR:HG21	1:58:A:ILE:HA	17	0.35
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	3	0.35
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	3	0.35
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	12	0.35
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	12	0.35
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	1	0.35
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	1	0.35
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	13	0.35
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	13	0.35
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	15	0.35
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	15	0.35
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG23	10	0.35
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	14	0.34
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	14	0.34
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	1	0.34
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	9	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	1	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	1	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	6	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	6	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	13	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	13	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	14	0.34
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	14	0.34
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	14	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	14	0.34
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	17	0.34
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	17	0.34
(1,2697)	1:69:B:THR:HG1	1:98:B:ILE:HA	2	0.34
(1,2574)	1:5:B:THR:HG21	1:83:B:PRO:HG3	3	0.34
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	8	0.34
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	12	0.34
(1,2327)	1:41:B:THR:HG1	1:17:B:THR:HG22	8	0.34
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	19	0.34
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	19	0.34
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	3	0.34
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	20	0.34
(1,2107)	1:98:B:ILE:HD12	1:102:B:ILE:HG13	6	0.34
(1,2107)	1:98:B:ILE:HD11	1:102:B:ILE:HG13	13	0.34
(1,2053)	1:69:B:THR:HG21	1:98:B:ILE:H	11	0.34
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	5	0.34
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	5	0.34
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	5	0.34
(1,1859)	1:79:B:ILE:HG23	1:78:B:LYS:HG2	9	0.34
(1,1853)	1:11:B:ASP:HB3	1:79:B:ILE:HG21	8	0.34
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	13	0.34
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG22	13	0.34
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG22	15	0.34
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	3	0.34
(1,1767)	1:56:B:PRO:HA	1:66:B:ILE:HG21	18	0.34
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	5	0.34
(1,1726)	1:57:B:THR:HG1	1:64:B:ASP:HB3	11	0.34
(1,1722)	1:64:B:ASP:HB2	1:43:B:ILE:HG13	1	0.34
(1,1693)	1:57:B:THR:HG1	1:58:B:ILE:HA	20	0.34
(1,1688)	1:57:B:THR:HG1	1:57:B:THR:HA	6	0.34
(1,1686)	1:57:B:THR:HG21	1:43:B:ILE:HB	17	0.34
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG21	10	0.34
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	1	0.34
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	1	0.34
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	9	0.34
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	9	0.34
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	3	0.34
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	3	0.34
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	19	0.34
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	19	0.34
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	9	0.34
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1380)	1:103:A:THR:HG21	1:105:A:ILE:HB	7	0.34
(1,1313)	1:69:A:THR:HG22	1:98:A:ILE:HA	13	0.34
(1,1190)	1:5:A:THR:HG23	1:83:A:PRO:HG3	3	0.34
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	13	0.34
(1,1048)	1:41:A:THR:HG21	1:66:A:ILE:HB	6	0.34
(1,1048)	1:41:A:THR:HG21	1:66:A:ILE:HB	9	0.34
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG21	3	0.34
(1,723)	1:98:A:ILE:HD11	1:102:A:ILE:HG13	15	0.34
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG23	11	0.34
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	14	0.34
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	20	0.34
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG21	8	0.34
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD11	13	0.34
(1,309)	1:57:A:THR:HG21	1:58:A:ILE:HA	6	0.34
(1,309)	1:57:A:THR:HG22	1:58:A:ILE:HA	8	0.34
(1,304)	1:57:A:THR:HG1	1:57:A:THR:HA	8	0.34
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	10	0.34
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	2	0.34
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	2	0.34
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	7	0.34
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	7	0.34
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	5	0.34
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	5	0.34
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB2	12	0.34
(1,70)	1:15:A:ALA:HA	1:18:A:TYR:HB3	12	0.34
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	2	0.33
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	2	0.33
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	9	0.33
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	9	0.33
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	3	0.33
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	3	0.33
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	15	0.33
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	15	0.33
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	16	0.33
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	16	0.33
(1,2847)	1:10:A:LYS:H	1:10:A:LYS:HG2	5	0.33
(1,2847)	1:10:A:LYS:H	1:10:A:LYS:HG3	5	0.33
(1,2803)	1:60:A:ILE:H	1:58:A:ILE:HG13	19	0.33
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	6	0.33
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	6	0.33
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	11	0.33
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	11	0.33
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	11	0.33
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	11	0.33
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	11	0.33
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	11	0.33
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	11	0.33
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	11	0.33
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	11	0.33
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	11	0.33
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	11	0.33
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	11	0.33
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	11	0.33
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	11	0.33
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	11	0.33
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	11	0.33
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	11	0.33
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	11	0.33
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	11	0.33
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	11	0.33
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	11	0.33
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	11	0.33
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	11	0.33
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	11	0.33
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	11	0.33
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	11	0.33
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	11	0.33
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	11	0.33
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	11	0.33
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	11	0.33
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	11	0.33
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	11	0.33
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	11	0.33
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	11	0.33
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	11	0.33
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	3	0.33
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	14	0.33
(1,1965)	1:58:B:ILE:HG21	1:90:B:PHE:HD1	5	0.33
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	1	0.33
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	1	0.33
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	1	0.33
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	4	0.33
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	4	0.33
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	7	0.33
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	7	0.33
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	7	0.33
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	7	0.33
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	7	0.33
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	7	0.33
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	8	0.33
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	1	0.33
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	7	0.33
(1,1693)	1:57:B:THR:HG1	1:58:B:ILE:HA	17	0.33
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	9	0.33
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	9	0.33
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	9	0.33
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	9	0.33
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	19	0.33
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	19	0.33
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	19	0.33
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	19	0.33
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	15	0.33
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	15	0.33
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	20	0.33
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	20	0.33
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	8	0.33
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	8	0.33
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	12	0.33
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	12	0.33
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB2	14	0.33
(1,1454)	1:15:B:ALA:HA	1:18:B:TYR:HB3	14	0.33
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	9	0.33
(1,1313)	1:69:A:THR:HG1	1:98:A:ILE:HA	3	0.33
(1,1190)	1:5:A:THR:HG23	1:83:A:PRO:HG3	16	0.33
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	17	0.33
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	17	0.33
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	2	0.33
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	8	0.33
(1,723)	1:98:A:ILE:HD13	1:102:A:ILE:HG13	19	0.33
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	18	0.33
(1,575)	1:89:A:THR:HG23	1:87:A:LEU:HB2	2	0.33
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	20	0.33
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	20	0.33
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	20	0.33
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	20	0.33
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	20	0.33
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	20	0.33
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	20	0.33
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	20	0.33
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	20	0.33
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	20	0.33
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	20	0.33
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	6	0.33
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	1	0.33
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	1	0.33
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	1	0.33
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	1	0.33
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	1	0.33
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	1	0.33
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	2	0.33
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	10	0.33
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	13	0.33
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD12	16	0.33
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	17	0.33
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	14	0.33
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	14	0.33
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	1	0.33
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	1	0.33
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	5	0.33
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	5	0.33
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	15	0.33
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	15	0.33
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	5	0.32
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	5	0.32
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	7	0.32
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	7	0.32
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	8	0.32
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	8	0.32
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	16	0.32
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	16	0.32
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	8	0.32
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	8	0.32
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	18	0.32
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	18	0.32
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	3	0.32
(1,2921)	1:58:A:ILE:H	1:58:A:ILE:HG21	20	0.32
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	8	0.32
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	8	0.32
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	12	0.32
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	12	0.32
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	16	0.32
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	16	0.32
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	19	0.32
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	19	0.32
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	20	0.32
(1,2432)	1:41:B:THR:HG21	1:66:B:ILE:HB	8	0.32
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	9	0.32
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	17	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	8	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	8	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	11	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	11	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	18	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	18	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	20	0.32
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	20	0.32
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	1	0.32
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	13	0.32
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG21	17	0.32
(1,1978)	1:89:B:THR:HG1	1:90:B:PHE:HB2	15	0.32
(1,1859)	1:79:B:ILE:HG23	1:78:B:LYS:HG2	2	0.32
(1,1800)	1:37:B:VAL:HG22	1:73:B:THR:HG22	1	0.32
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	8	0.32
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	15	0.32
(1,1695)	1:58:B:ILE:HG12	1:57:B:THR:HB	5	0.32
(1,1650)	1:44:B:GLU:HB2	1:43:B:ILE:HG13	15	0.32
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	6	0.32
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	6	0.32
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	6	0.32
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	6	0.32
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	5	0.32
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	5	0.32
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	4	0.32
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	4	0.32
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	14	0.32
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	15	0.32
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	15	0.32
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	8	0.32
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	8	0.32
(1,1356)	1:102:A:ILE:HG22	1:101:A:LEU:HG	10	0.32
(1,1048)	1:41:A:THR:HG22	1:66:A:ILE:HB	1	0.32
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	8	0.32
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	3	0.32
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	3	0.32
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	13	0.32
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	13	0.32
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	18	0.32
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	18	0.32
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	17	0.32
(1,730)	1:103:A:THR:HG22	1:99:A:ASP:HB2	2	0.32
(1,730)	1:103:A:THR:HG23	1:99:A:ASP:HB2	15	0.32
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	4	0.32
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	4	0.32
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	4	0.32
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	4	0.32
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	4	0.32
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	4	0.32
(1,669)	1:69:A:THR:HG23	1:98:A:ILE:H	15	0.32
(1,564)	1:87:A:LEU:HD23	1:60:A:ILE:HG23	16	0.32
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	12	0.32
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	12	0.32
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	12	0.32
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG21	8	0.32
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	5	0.32
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	5	0.32
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	5	0.32
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	5	0.32
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	5	0.32
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	5	0.32
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	15	0.32
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD2	19	0.32
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	1	0.32
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	8	0.32
(1,341)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	14	0.32
(1,309)	1:57:A:THR:HG22	1:58:A:ILE:HA	9	0.32
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	2	0.32
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	2	0.32
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	2	0.32
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	16	0.32
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	16	0.32
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	16	0.32
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	16	0.32
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	11	0.32
(1,187)	1:34:A:THR:HG22	1:34:A:THR:HA	13	0.32
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	10	0.32
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	10	0.32
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	11	0.32
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	11	0.32
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	16	0.32
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	16	0.32
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	18	0.32
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	18	0.32
(1,38)	1:8:A:LYS:HD2	1:8:A:LYS:HA	5	0.32
(1,38)	1:8:A:LYS:HD3	1:8:A:LYS:HA	5	0.32
(1,3129)	1:18:B:TYR:H	1:17:B:THR:HB	13	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	3	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	3	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	12	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	12	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	13	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	13	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	15	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	15	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	17	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	17	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	20	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	20	0.31
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	10	0.31
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	10	0.31
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	16	0.31
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	16	0.31
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	19	0.31
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	19	0.31
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	1	0.31
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	1	0.31
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	6	0.31
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	6	0.31
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	18	0.31
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	9	0.31
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	9	0.31
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	19	0.31
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	19	0.31
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	6	0.31
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	6	0.31
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	18	0.31
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	18	0.31
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	20	0.31
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	20	0.31
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	8	0.31
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	8	0.31
(1,2671)	1:90:B:PHE:HB3	1:94:B:ILE:HG13	2	0.31
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	11	0.31
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	7	0.31
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	7	0.31
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	7	0.31
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	7	0.31
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	7	0.31
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	7	0.31
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	7	0.31
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	7	0.31
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	7	0.31
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	7	0.31
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	7	0.31
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	7	0.31
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	7	0.31
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	7	0.31
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	7	0.31
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	7	0.31
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	7	0.31
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	7	0.31
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	7	0.31
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	7	0.31
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	7	0.31
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	7	0.31
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	7	0.31
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	7	0.31
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	7	0.31
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	7	0.31
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	7	0.31
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	7	0.31
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	7	0.31
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	7	0.31
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	7	0.31
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	7	0.31
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	7	0.31
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	7	0.31
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	7	0.31
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	10	0.31
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	10	0.31
(1,2114)	1:103:B:THR:HG22	1:99:B:ASP:HB2	14	0.31
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	5	0.31
(1,2085)	1:69:B:THR:HG23	1:101:B:LEU:HB3	1	0.31
(1,2073)	1:69:B:THR:HG1	1:100:B:PHE:HD2	18	0.31
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	16	0.31
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	1	0.31
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	1	0.31
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	2	0.31
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	2	0.31
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	2	0.31
(1,1853)	1:11:B:ASP:HB2	1:79:B:ILE:HG21	15	0.31
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	18	0.31
(1,1725)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	8	0.31
(1,1695)	1:58:B:ILE:HG21	1:57:B:THR:HB	10	0.31
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	2	0.31
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	8	0.31
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	2	0.31
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	2	0.31
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	2	0.31
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	2	0.31
(1,1571)	1:34:B:THR:HG1	1:34:B:THR:HA	2	0.31
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	3	0.31
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	3	0.31
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	7	0.31
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	7	0.31
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	8	0.31
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	8	0.31
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	1	0.31
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	1	0.31
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	8	0.31
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	13	0.31
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	13	0.31
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	18	0.31
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	18	0.31
(1,1450)	1:17:B:THR:HG23	1:16:B:LYS:HB2	13	0.31
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	8	0.31
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	16	0.31
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	16	0.31
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	15	0.31
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	13	0.31
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	13	0.31
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	13	0.31
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	19	0.31
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	19	0.31
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	19	0.31
(1,669)	1:69:A:THR:HG22	1:98:A:ILE:H	8	0.31
(1,669)	1:69:A:THR:HG23	1:98:A:ILE:H	20	0.31
(1,594)	1:89:A:THR:HG23	1:90:A:PHE:HB2	16	0.31
(1,581)	1:58:A:ILE:HG23	1:90:A:PHE:HD1	10	0.31
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	4	0.31
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	4	0.31
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	4	0.31
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	10	0.31
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	10	0.31
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	10	0.31
(1,475)	1:79:A:ILE:HG22	1:78:A:LYS:HG2	1	0.31
(1,475)	1:79:A:ILE:HG23	1:78:A:LYS:HG2	11	0.31
(1,469)	1:11:A:ASP:HB2	1:79:A:ILE:HG21	19	0.31
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG22	13	0.31
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG21	14	0.31
(1,417)	1:37:A:VAL:HG22	1:73:A:THR:HG1	5	0.31
(1,417)	1:37:A:VAL:HG23	1:73:A:THR:HG21	19	0.31
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	12	0.31
(1,380)	1:66:A:ILE:HG21	1:43:A:ILE:HD11	6	0.31
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	6	0.31
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	6	0.31
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	19	0.31
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	19	0.31
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG21	4	0.31
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	4	0.3
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	4	0.3
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	11	0.3
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	7	0.3
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	7	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	3	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	3	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	4	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	4	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	7	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	7	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	11	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	11	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	18	0.3
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	18	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	2	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	2	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	8	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	8	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	11	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	11	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	12	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	12	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	17	0.3
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	17	0.3
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	13	0.3
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	13	0.3
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	9	0.3
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	9	0.3
(1,2764)	1:103:B:THR:HG21	1:105:B:ILE:HB	7	0.3
(1,2574)	1:5:B:THR:HG22	1:83:B:PRO:HG3	7	0.3
(1,2574)	1:5:B:THR:HG23	1:83:B:PRO:HG3	10	0.3
(1,2574)	1:5:B:THR:HG23	1:83:B:PRO:HG3	18	0.3
(1,2413)	1:43:B:ILE:HG22	1:64:B:ASP:HB3	18	0.3
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	14	0.3
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	14	0.3
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	10	0.3
(1,2114)	1:103:B:THR:HG23	1:99:B:ASP:HB2	12	0.3
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	13	0.3
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	13	0.3
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	13	0.3
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	19	0.3
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	19	0.3
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2053)	1:69:B:THR:HG22	1:98:B:ILE:H	15	0.3
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG12	10	0.3
(1,1965)	1:58:B:ILE:HG21	1:90:B:PHE:HD2	1	0.3
(1,1959)	1:89:B:THR:HG21	1:87:B:LEU:HB2	4	0.3
(1,1948)	1:87:B:LEU:HD13	1:60:B:ILE:HG21	13	0.3
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD11	19	0.3
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	7	0.3
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	7	0.3
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	7	0.3
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	7	0.3
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	7	0.3
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	7	0.3
(1,1859)	1:79:B:ILE:HG23	1:78:B:LYS:HG2	17	0.3
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	5	0.3
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	5	0.3
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	5	0.3
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	5	0.3
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	5	0.3
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	5	0.3
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG21	4	0.3
(1,1794)	1:69:B:THR:HG1	1:56:B:PRO:HD3	3	0.3
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	4	0.3
(1,1693)	1:57:B:THR:HG22	1:58:B:ILE:HA	14	0.3
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	8	0.3
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	8	0.3
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	8	0.3
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	8	0.3
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	14	0.3
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	14	0.3
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	17	0.3
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	13	0.3
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	13	0.3
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	9	0.3
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	9	0.3
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	16	0.3
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	16	0.3
(1,1356)	1:102:A:ILE:HG12	1:101:A:LEU:HG	20	0.3
(1,1288)	1:94:A:ILE:HG12	1:90:A:PHE:HB3	1	0.3
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	2	0.3
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	11	0.3
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	14	0.3
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	14	0.3
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	14	0.3
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	14	0.3
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	14	0.3
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	14	0.3
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	14	0.3
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	14	0.3
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	14	0.3
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	14	0.3
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	14	0.3
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	14	0.3
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	14	0.3
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	14	0.3
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	14	0.3
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	14	0.3
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	14	0.3
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	14	0.3
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	14	0.3
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	14	0.3
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	14	0.3
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	14	0.3
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	14	0.3
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	14	0.3
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	14	0.3
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	14	0.3
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	14	0.3
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	14	0.3
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	14	0.3
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	14	0.3
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	14	0.3
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	14	0.3
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	14	0.3
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	14	0.3
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	14	0.3
(1,1048)	1:41:A:THR:HG22	1:66:A:ILE:HB	11	0.3
(1,1048)	1:41:A:THR:HG22	1:66:A:ILE:HB	18	0.3
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	15	0.3
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	15	0.3
(1,730)	1:103:A:THR:HG22	1:99:A:ASP:HB2	10	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	15	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	15	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	15	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	15	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	15	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	20	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	20	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	20	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	20	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	20	0.3
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	20	0.3
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	4	0.3
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	4	0.3
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	4	0.3
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	10	0.3
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	10	0.3
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	10	0.3
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	2	0.3
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	2	0.3
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	2	0.3
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	2	0.3
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	2	0.3
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	2	0.3
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	14	0.3
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	14	0.3
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	14	0.3
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	14	0.3
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	14	0.3
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	14	0.3
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	18	0.3
(1,475)	1:79:A:ILE:HG23	1:78:A:LYS:HG2	8	0.3
(1,475)	1:79:A:ILE:HG23	1:78:A:LYS:HG2	9	0.3
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG22	10	0.3
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	11	0.3
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	4	0.3
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	10	0.3
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	7	0.3
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	7	0.3
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	7	0.3
(1,311)	1:58:A:ILE:HG21	1:57:A:THR:HB	12	0.3
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	7	0.3
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	7	0.3
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	7	0.3
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	13	0.3
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	13	0.3
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	13	0.3
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	13	0.3
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG21	3	0.3
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	12	0.3
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	12	0.3
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	3	0.3
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	3	0.3
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	18	0.3
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	12	0.3
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	12	0.3
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	17	0.3
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	17	0.3
(1,66)	1:17:A:THR:HG1	1:16:A:LYS:HB2	11	0.3
(1,3179)	1:58:B:ILE:H	1:58:B:ILE:HG21	16	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	1	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	1	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	10	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	10	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	14	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	14	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	18	0.29
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	18	0.29
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	2	0.29
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	2	0.29
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	15	0.29
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	3	0.29
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	9	0.29
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	9	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	5	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	5	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	10	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	10	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	16	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	16	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	17	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	17	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	20	0.29
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	20	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	3	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	9	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	9	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	10	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	10	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	15	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	15	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	19	0.29
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	19	0.29
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	12	0.29
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	12	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	10	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	10	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	11	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	11	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	15	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	15	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	20	0.29
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	20	0.29
(1,2697)	1:69:B:THR:HG1	1:98:B:ILE:HA	8	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	6	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	6	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	6	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	6	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	6	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	6	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	6	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	6	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	6	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	6	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	6	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	6	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	6	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	6	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	6	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	6	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	6	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	6	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	6	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	6	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	6	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	6	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	6	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	6	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	6	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	6	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	6	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	6	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	6	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	6	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	6	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	6	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	6	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	6	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	6	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	16	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	16	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	16	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	16	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	16	0.29
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	16	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	16	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	16	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	16	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	16	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	16	0.29
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	16	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	16	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	16	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	16	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	16	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	16	0.29
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	16	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	16	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	16	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	16	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	16	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	16	0.29
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	16	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	16	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	16	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	16	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	16	0.29
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	16	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	16	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	16	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	16	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	16	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	16	0.29
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	16	0.29
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	1	0.29
(1,2376)	1:58:B:ILE:HG23	1:56:B:PRO:HB2	5	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	3	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	3	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	6	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	6	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	15	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	15	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	16	0.29
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	16	0.29
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	1	0.29
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	1	0.29
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	1	0.29
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	3	0.29
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	3	0.29
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	3	0.29
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	6	0.29
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	6	0.29
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	6	0.29
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	10	0.29
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	10	0.29
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	10	0.29
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	15	0.29
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	15	0.29
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	15	0.29
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	17	0.29
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	17	0.29
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	17	0.29
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	20	0.29
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	20	0.29
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	20	0.29
(1,1978)	1:89:B:THR:HG21	1:90:B:PHE:HB2	6	0.29
(1,1948)	1:87:B:LEU:HD11	1:60:B:ILE:HG23	19	0.29
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	7	0.29
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	7	0.29
(1,1859)	1:79:B:ILE:HG22	1:78:B:LYS:HG2	4	0.29
(1,1859)	1:79:B:ILE:HG21	1:78:B:LYS:HG2	12	0.29
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG21	2	0.29
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG1	13	0.29
(1,1794)	1:69:B:THR:HG1	1:56:B:PRO:HD3	19	0.29
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	3	0.29
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	7	0.29
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	10	0.29
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	13	0.29
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD12	6	0.29
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	16	0.29
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	5	0.29
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	5	0.29
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	5	0.29
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	5	0.29
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	15	0.29
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	15	0.29
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	15	0.29
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	15	0.29
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	6	0.29
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	6	0.29
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	19	0.29
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	19	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	2	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	2	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	10	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	10	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	11	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	11	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	20	0.29
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	20	0.29
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	3	0.29
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	3	0.29
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	14	0.29
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	14	0.29
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	17	0.29
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	17	0.29
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	2	0.29
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	2	0.29
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	6	0.29
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	15	0.29
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	15	0.29
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	14	0.29
(1,1288)	1:94:A:ILE:HG13	1:90:A:PHE:HB3	18	0.29
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	16	0.29
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	16	0.29
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	16	0.29
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	16	0.29
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	16	0.29
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	16	0.29
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	16	0.29
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	16	0.29
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	16	0.29
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	16	0.29
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	16	0.29
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	16	0.29
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	16	0.29
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	16	0.29
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	16	0.29
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	16	0.29
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	16	0.29
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	16	0.29
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	16	0.29
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	16	0.29
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	16	0.29
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	16	0.29
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	16	0.29
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	16	0.29
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	16	0.29
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	16	0.29
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	16	0.29
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	16	0.29
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	16	0.29
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	16	0.29
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	16	0.29
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	16	0.29
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	16	0.29
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	16	0.29
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	16	0.29
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	16	0.29
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	14	0.29
(1,1048)	1:41:A:THR:HG21	1:66:A:ILE:HB	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	2	0.29
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	2	0.29
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	2	0.29
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	14	0.29
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	14	0.29
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	3	0.29
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	12	0.29
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	3	0.29
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	3	0.29
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	3	0.29
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	3	0.29
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	3	0.29
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	3	0.29
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	13	0.29
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	5	0.29
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	5	0.29
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	5	0.29
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	9	0.29
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	9	0.29
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	9	0.29
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	15	0.29
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	15	0.29
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	15	0.29
(1,594)	1:89:A:THR:HG21	1:90:A:PHE:HB2	7	0.29
(1,594)	1:89:A:THR:HG22	1:90:A:PHE:HB2	11	0.29
(1,575)	1:89:A:THR:HG23	1:87:A:LEU:HB2	17	0.29
(1,475)	1:79:A:ILE:HG23	1:78:A:LYS:HG2	4	0.29
(1,475)	1:79:A:ILE:HG23	1:78:A:LYS:HG2	10	0.29
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	20	0.29
(1,361)	1:43:A:ILE:HG13	1:65:A:PHE:HB3	16	0.29
(1,341)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	1	0.29
(1,309)	1:57:A:THR:HG22	1:58:A:ILE:HA	5	0.29
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	3	0.29
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	1	0.29
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	1	0.29
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	1	0.29
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	1	0.29
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	12	0.29
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	12	0.29
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	12	0.29
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	12	0.29
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	15	0.29
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	15	0.29
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	15	0.29
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	5	0.29
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	5	0.29
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	12	0.29
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	12	0.29
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	2	0.29
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	2	0.29
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	4	0.29
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	4	0.29
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	15	0.29
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	15	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	3	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	3	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	7	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	7	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	8	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	8	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	15	0.29
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	15	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	10	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	10	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	11	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	11	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	13	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	13	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	16	0.29
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	16	0.29
(1,3179)	1:58:B:ILE:H	1:58:B:ILE:HG21	13	0.28
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	18	0.28
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	18	0.28
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	13	0.28
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	13	0.28
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	5	0.28
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	5	0.28
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	12	0.28
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	12	0.28
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	15	0.28
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	15	0.28
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	19	0.28
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	18	0.28
(1,2921)	1:58:A:ILE:H	1:58:A:ILE:HG21	5	0.28
(1,2921)	1:58:A:ILE:H	1:58:A:ILE:HG21	18	0.28
(1,2847)	1:10:A:LYS:H	1:10:A:LYS:HG2	1	0.28
(1,2847)	1:10:A:LYS:H	1:10:A:LYS:HG3	1	0.28
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	7	0.28
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	7	0.28
(1,2758)	1:103:B:THR:HG23	1:102:B:ILE:HG23	3	0.28
(1,2758)	1:103:B:THR:HG22	1:102:B:ILE:HG23	12	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	14	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	14	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	14	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	14	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	14	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	14	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	14	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	14	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	14	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	14	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	14	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	14	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	14	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	14	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	14	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	14	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	14	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	14	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	14	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	14	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	14	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	14	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	14	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	14	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	14	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	14	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	14	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	14	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	14	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	14	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	14	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	14	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	14	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	14	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	14	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	19	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	19	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	19	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	19	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	19	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	19	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	19	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	19	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	19	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	19	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	19	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	19	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	19	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	19	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	19	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	19	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	19	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	19	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	19	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	19	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	19	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	19	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	19	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	19	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	19	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	19	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	19	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	19	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	19	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	19	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	19	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	19	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	19	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	19	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	19	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	19	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	20	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	20	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	20	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	20	0.28
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	20	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	20	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	20	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	20	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	20	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	20	0.28
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	20	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	20	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	20	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	20	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	20	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	20	0.28
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	20	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	20	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	20	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	20	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	20	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	20	0.28
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	20	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	20	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	20	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	20	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	20	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	20	0.28
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	20	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	20	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	20	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	20	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	20	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	20	0.28
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	20	0.28
(1,2117)	1:103:B:THR:HG23	1:102:B:ILE:HB	10	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	2	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	2	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	2	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	2	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	2	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	2	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	8	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	8	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	8	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	8	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	8	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	13	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	13	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	13	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	13	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	13	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	13	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	14	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	14	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	14	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	14	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	14	0.28
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	14	0.28
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	5	0.28
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	5	0.28
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	5	0.28
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	8	0.28
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	8	0.28
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	8	0.28
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	11	0.28
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	11	0.28
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	11	0.28
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	14	0.28
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	14	0.28
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	14	0.28
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	16	0.28
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	16	0.28
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	16	0.28
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	3	0.28
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	3	0.28
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	12	0.28
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	12	0.28
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	12	0.28
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	12	0.28
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	12	0.28
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	12	0.28
(1,1948)	1:87:B:LEU:HD13	1:60:B:ILE:HG21	7	0.28
(1,1948)	1:87:B:LEU:HD11	1:60:B:ILE:HG23	9	0.28
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	7	0.28
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	7	0.28
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	7	0.28
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	7	0.28
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	7	0.28
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	7	0.28
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	7	0.28
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	7	0.28
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	7	0.28
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	7	0.28
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	7	0.28
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	15	0.28
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	15	0.28
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	15	0.28
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	15	0.28
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	15	0.28
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	15	0.28
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	15	0.28
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	15	0.28
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	15	0.28
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	15	0.28
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	15	0.28
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	15	0.28
(1,1859)	1:79:B:ILE:HG23	1:78:B:LYS:HG2	5	0.28
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG1	20	0.28
(1,1800)	1:37:B:VAL:HG23	1:73:B:THR:HG22	5	0.28
(1,1794)	1:69:B:THR:HG22	1:56:B:PRO:HD3	12	0.28
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	3	0.28
(1,1745)	1:43:B:ILE:HG13	1:65:B:PHE:HB3	9	0.28
(1,1693)	1:57:B:THR:HG23	1:58:B:ILE:HA	11	0.28
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	13	0.28
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	7	0.28
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	7	0.28
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	17	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	2	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	2	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	5	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	5	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	14	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	14	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	20	0.28
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	3	0.28
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	3	0.28
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	7	0.28
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	7	0.28
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	17	0.28
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	17	0.28
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	18	0.28
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	18	0.28
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	2	0.28
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	2	0.28
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	16	0.28
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	16	0.28
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	17	0.28
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	17	0.28
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	14	0.28
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	14	0.28
(1,1376)	1:103:A:THR:HG23	1:103:A:THR:HA	19	0.28
(1,1374)	1:103:A:THR:HG1	1:102:A:ILE:HG21	12	0.28
(1,1190)	1:5:A:THR:HG21	1:83:A:PRO:HG3	7	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	2	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	2	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	2	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	2	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	2	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	2	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	2	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	2	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	2	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	2	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	2	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	2	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	2	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	2	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	2	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	2	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	2	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	2	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	2	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	2	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	2	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	2	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	2	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	2	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	2	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	2	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	2	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	2	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	2	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	2	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	2	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	2	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	2	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	2	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	2	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	4	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	4	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	4	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	4	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	4	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	4	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	4	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	4	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	4	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	4	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	4	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	4	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	4	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	4	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	4	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	4	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	4	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	4	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	4	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	4	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	4	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	4	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	4	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	4	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	4	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	4	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	4	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	4	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	4	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	4	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	4	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	4	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	4	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	4	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	4	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	10	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	10	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	10	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	10	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	10	0.28
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	10	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	10	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	10	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	10	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	10	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	10	0.28
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	10	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	10	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	10	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	10	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	10	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	10	0.28
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	10	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	10	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	10	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	10	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	10	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	10	0.28
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	10	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	10	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	10	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	10	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	10	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	10	0.28
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	10	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	10	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	10	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	10	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	10	0.28
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	10	0.28
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	6	0.28
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	6	0.28
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	19	0.28
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	19	0.28
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	20	0.28
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	20	0.28
(1,733)	1:103:A:THR:HG23	1:102:A:ILE:HB	11	0.28
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	14	0.28
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	1	0.28
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	1	0.28
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	1	0.28
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	1	0.28
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	1	0.28
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	1	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	2	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	2	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	2	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	3	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	3	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	3	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	6	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	6	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	6	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	7	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	7	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	7	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	8	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	8	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	8	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	11	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	11	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	11	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	14	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	14	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	14	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	16	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	16	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	16	0.28
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	17	0.28
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	17	0.28
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	3	0.28
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	3	0.28
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG21	19	0.28
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	5	0.28
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	5	0.28
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	5	0.28
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	5	0.28
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	5	0.28
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	5	0.28
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	5	0.28
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	5	0.28
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	5	0.28
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	5	0.28
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	5	0.28
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	5	0.28
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	7	0.28
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	7	0.28
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	7	0.28
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	7	0.28
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	7	0.28
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	7	0.28
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	7	0.28
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	7	0.28
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	7	0.28
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	7	0.28
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	7	0.28
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	7	0.28
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG11	13	0.28
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG12	13	0.28
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG13	13	0.28
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG21	13	0.28
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG22	13	0.28
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG23	13	0.28
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG11	13	0.28
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG12	13	0.28
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG13	13	0.28
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG21	13	0.28
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG22	13	0.28
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG23	13	0.28
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG11	13	0.28
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG12	13	0.28
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG13	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG21	13	0.28
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG22	13	0.28
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG23	13	0.28
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	10	0.28
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	10	0.28
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	10	0.28
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	10	0.28
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	10	0.28
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	10	0.28
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG21	16	0.28
(1,417)	1:37:A:VAL:HG22	1:73:A:THR:HG23	18	0.28
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	14	0.28
(1,341)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	12	0.28
(1,338)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	14	0.28
(1,278)	1:48:A:LYS:HD2	1:43:A:ILE:HG21	18	0.28
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	9	0.28
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	1	0.28
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	1	0.28
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	7	0.28
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	7	0.28
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	19	0.28
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	2	0.28
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	2	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	9	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	9	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	17	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	17	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	18	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	18	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	20	0.28
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	20	0.28
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	2	0.28
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	2	0.28
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	8	0.28
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	8	0.28
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	9	0.28
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	9	0.28
(1,3050)	1:36:B:LEU:H	1:24:B:VAL:H	3	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	1	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	1	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	4	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	10	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	10	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	13	0.27
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	13	0.27
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	1	0.27
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	2	0.27
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	4	0.27
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	4	0.27
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	4	0.27
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	4	0.27
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	4	0.27
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	4	0.27
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	12	0.27
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	12	0.27
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	9	0.27
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	15	0.27
(1,2764)	1:103:B:THR:HG21	1:105:B:ILE:HB	6	0.27
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	5	0.27
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	5	0.27
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	5	0.27
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	5	0.27
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	5	0.27
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	5	0.27
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	5	0.27
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	5	0.27
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	5	0.27
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	5	0.27
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	5	0.27
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	5	0.27
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	5	0.27
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	5	0.27
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	5	0.27
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	5	0.27
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	5	0.27
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	5	0.27
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	5	0.27
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	5	0.27
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	5	0.27
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	5	0.27
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	5	0.27
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	5	0.27
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	5	0.27
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	5	0.27
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	5	0.27
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	5	0.27
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	5	0.27
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	5	0.27
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	5	0.27
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	5	0.27
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	5	0.27
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	5	0.27
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	5	0.27
(1,2432)	1:41:B:THR:HG21	1:66:B:ILE:HB	10	0.27
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	16	0.27
(1,2117)	1:103:B:THR:HG22	1:102:B:ILE:HB	19	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	6	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	6	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	6	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	6	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	6	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	6	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	19	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	19	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	19	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	19	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	19	0.27
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	19	0.27
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	14	0.27
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	14	0.27
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	9	0.27
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	9	0.27
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	9	0.27
(1,2053)	1:69:B:THR:HG21	1:98:B:ILE:H	13	0.27
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	8	0.27
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	8	0.27
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	9	0.27
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	9	0.27
(1,1978)	1:89:B:THR:HG23	1:90:B:PHE:HB2	2	0.27
(1,1978)	1:89:B:THR:HG21	1:90:B:PHE:HB2	10	0.27
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	14	0.27
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	14	0.27
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	14	0.27
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	14	0.27
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	14	0.27
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	15	0.27
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	15	0.27
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	15	0.27
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	15	0.27
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	15	0.27
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	15	0.27
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	17	0.27
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	17	0.27
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	17	0.27
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	17	0.27
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	17	0.27
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	17	0.27
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	20	0.27
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	20	0.27
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	20	0.27
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	20	0.27
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	20	0.27
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	20	0.27
(1,1948)	1:87:B:LEU:HD22	1:60:B:ILE:HG21	11	0.27
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	15	0.27
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	15	0.27
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	15	0.27
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	15	0.27
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	15	0.27
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	15	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	5	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	5	0.27
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	5	0.27
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	5	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	5	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	5	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	5	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	5	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	5	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	5	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	5	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	5	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	6	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	6	0.27
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	6	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	6	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	6	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	6	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	6	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	6	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	6	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	6	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	6	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	12	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	12	0.27
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	12	0.27
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	12	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	12	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	12	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	12	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	12	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	12	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	12	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	12	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	12	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	17	0.27
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	17	0.27
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	17	0.27
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	17	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	17	0.27
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	17	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	17	0.27
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	17	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	17	0.27
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	17	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	17	0.27
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	17	0.27
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG11	8	0.27
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG12	8	0.27
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG13	8	0.27
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG21	8	0.27
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG22	8	0.27
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG23	8	0.27
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG11	8	0.27
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG12	8	0.27
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG13	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG21	8	0.27
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG22	8	0.27
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG23	8	0.27
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG11	8	0.27
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG12	8	0.27
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG13	8	0.27
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG21	8	0.27
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG22	8	0.27
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG23	8	0.27
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG22	11	0.27
(1,1800)	1:37:B:VAL:HG22	1:73:B:THR:HG23	6	0.27
(1,1794)	1:69:B:THR:HG1	1:56:B:PRO:HD3	5	0.27
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	5	0.27
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	17	0.27
(1,1722)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	8	0.27
(1,1696)	1:58:B:ILE:HG12	1:57:B:THR:HB	6	0.27
(1,1696)	1:58:B:ILE:HG13	1:57:B:THR:HB	13	0.27
(1,1695)	1:58:B:ILE:HG12	1:57:B:THR:HB	6	0.27
(1,1695)	1:58:B:ILE:HG13	1:57:B:THR:HB	13	0.27
(1,1693)	1:57:B:THR:HG22	1:58:B:ILE:HA	6	0.27
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG23	5	0.27
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	8	0.27
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	8	0.27
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	9	0.27
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	9	0.27
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	10	0.27
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	10	0.27
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	10	0.27
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	10	0.27
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	12	0.27
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	12	0.27
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	20	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	5	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	5	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	11	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	11	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	19	0.27
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	19	0.27
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD1	11	0.27
(1,1472)	1:7:B:TYR:HA	1:20:B:TYR:HD2	11	0.27
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	3	0.27
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	7	0.27
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	7	0.27
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	10	0.27
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	10	0.27
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	12	0.27
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	12	0.27
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	20	0.27
(1,1313)	1:69:A:THR:HG1	1:98:A:ILE:HA	2	0.27
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	5	0.27
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	5	0.27
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	5	0.27
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	5	0.27
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	5	0.27
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	5	0.27
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	5	0.27
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	5	0.27
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	5	0.27
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	5	0.27
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	5	0.27
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	5	0.27
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	5	0.27
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	5	0.27
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	5	0.27
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	5	0.27
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	5	0.27
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	5	0.27
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	5	0.27
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	5	0.27
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	5	0.27
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	5	0.27
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	5	0.27
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	5	0.27
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	5	0.27
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	5	0.27
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	5	0.27
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	5	0.27
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	5	0.27
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	5	0.27
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	5	0.27
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	5	0.27
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	5	0.27
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	5	0.27
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	5	0.27
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	13	0.27
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	11	0.27
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	19	0.27
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	19	0.27
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	20	0.27
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	20	0.27
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	20	0.27
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	9	0.27
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	9	0.27
(1,594)	1:89:A:THR:HG21	1:90:A:PHE:HB2	1	0.27
(1,594)	1:89:A:THR:HG21	1:90:A:PHE:HB2	10	0.27
(1,581)	1:58:A:ILE:HG21	1:90:A:PHE:HD1	16	0.27
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	2	0.27
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	2	0.27
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	2	0.27
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	2	0.27
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	2	0.27
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	2	0.27
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	5	0.27
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	5	0.27
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	5	0.27
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	5	0.27
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	5	0.27
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	5	0.27
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	9	0.27
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	9	0.27
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	9	0.27
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	9	0.27
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	9	0.27
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	9	0.27
(1,564)	1:87:A:LEU:HD11	1:60:A:ILE:HG21	18	0.27
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	9	0.27
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	9	0.27
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	9	0.27
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	9	0.27
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	9	0.27
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	9	0.27
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	9	0.27
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	9	0.27
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	9	0.27
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	9	0.27
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	9	0.27
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	12	0.27
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	12	0.27
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	12	0.27
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	12	0.27
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	12	0.27
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	12	0.27
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	12	0.27
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	12	0.27
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	12	0.27
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	12	0.27
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	12	0.27
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	12	0.27
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	11	0.27
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	11	0.27
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	12	0.27
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	12	0.27
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	11	0.27
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	11	0.27
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	11	0.27
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	4	0.27
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	4	0.27
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	4	0.27
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	4	0.27
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	4	0.27
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	4	0.27
(1,332)	1:61:A:ASP:HB3	1:60:A:ILE:HG13	9	0.27
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	5	0.27
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	5	0.27
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	5	0.27
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	5	0.27
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	6	0.27
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	6	0.27
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	4	0.27
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	8	0.27
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	5	0.27
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	5	0.27
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	7	0.27
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	7	0.27
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	7	0.27
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	10	0.27
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	10	0.27
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	13	0.27
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	13	0.27
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	4	0.27
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	4	0.27
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	14	0.27
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	14	0.27
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	10	0.26
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	7	0.26
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	7	0.26
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB2	6	0.26
(1,3081)	1:88:B:SER:H	1:87:B:LEU:HB3	6	0.26
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	7	0.26
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	7	0.26
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	9	0.26
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	9	0.26
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	13	0.26
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	13	0.26
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	5	0.26
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	5	0.26
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	5	0.26
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	16	0.26
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	16	0.26
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	9	0.26
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	12	0.26
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	6	0.26
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	10	0.26
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	10	0.26
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	10	0.26
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	20	0.26
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB3	13	0.26
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	7	0.26
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	7	0.26
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG2	13	0.26
(1,2156)	1:10:B:LYS:HA	1:10:B:LYS:HG3	13	0.26
(1,2117)	1:103:B:THR:HG22	1:102:B:ILE:HB	11	0.26
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	17	0.26
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	17	0.26
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	17	0.26
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	17	0.26
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	17	0.26
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	13	0.26
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	13	0.26
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	2	0.26
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	2	0.26
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	2	0.26
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	7	0.26
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	7	0.26
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	7	0.26
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	18	0.26
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	18	0.26
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	18	0.26
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	5	0.26
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG12	1	0.26
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	18	0.26
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	18	0.26
(1,1959)	1:89:B:THR:HG21	1:87:B:LEU:HB2	18	0.26
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	1	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	1	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	1	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	1	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	1	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	1	0.26
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	3	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	3	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	3	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	3	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	3	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	3	0.26
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	4	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	4	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	4	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	4	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	4	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	4	0.26
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	8	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	8	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	8	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	8	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	8	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	10	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	10	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	10	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	10	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	10	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	10	0.26
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	11	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	11	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	11	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	11	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	11	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	11	0.26
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	19	0.26
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	19	0.26
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	19	0.26
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	19	0.26
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	19	0.26
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	19	0.26
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG21	17	0.26
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	11	0.26
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	11	0.26
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	11	0.26
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	11	0.26
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	11	0.26
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	11	0.26
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	4	0.26
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	4	0.26
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	4	0.26
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	4	0.26
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	4	0.26
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	4	0.26
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	4	0.26
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	4	0.26
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	4	0.26
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	4	0.26
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	4	0.26
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	4	0.26
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	13	0.26
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	13	0.26
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	13	0.26
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	13	0.26
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	13	0.26
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	13	0.26
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	13	0.26
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	13	0.26
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	13	0.26
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	13	0.26
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	13	0.26
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	18	0.26
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	18	0.26
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	18	0.26
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	18	0.26
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	18	0.26
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	18	0.26
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	18	0.26
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	18	0.26
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	18	0.26
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	18	0.26
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	18	0.26
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	18	0.26
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	4	0.26
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	4	0.26
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	9	0.26
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	9	0.26
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	17	0.26
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	17	0.26
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	6	0.26
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	6	0.26
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	6	0.26
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	6	0.26
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	6	0.26
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	6	0.26
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	16	0.26
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	16	0.26
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	16	0.26
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	16	0.26
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	16	0.26
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	16	0.26
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	19	0.26
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	19	0.26
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	19	0.26
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	19	0.26
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	19	0.26
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	20	0.26
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	20	0.26
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	20	0.26
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	20	0.26
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	20	0.26
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	20	0.26
(1,1767)	1:56:B:PRO:HA	1:66:B:ILE:HG21	8	0.26
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD11	14	0.26
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD13	16	0.26
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	18	0.26
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	19	0.26
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	4	0.26
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	4	0.26
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	4	0.26
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	4	0.26
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	18	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	7	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	7	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	11	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	11	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	13	0.26
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	13	0.26
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	8	0.26
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	8	0.26
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	13	0.26
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	13	0.26
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	6	0.26
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	6	0.26
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	12	0.26
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	12	0.26
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	18	0.26
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	18	0.26
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	6	0.26
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	6	0.26
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	19	0.26
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	19	0.26
(1,1380)	1:103:A:THR:HG23	1:105:A:ILE:HB	9	0.26
(1,1380)	1:103:A:THR:HG21	1:105:A:ILE:HB	16	0.26
(1,1048)	1:41:A:THR:HG21	1:66:A:ILE:HB	4	0.26
(1,733)	1:103:A:THR:HG21	1:102:A:ILE:HB	6	0.26
(1,733)	1:103:A:THR:HG23	1:102:A:ILE:HB	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:103:A:THR:HG23	1:99:A:ASP:HB2	18	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	9	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	9	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	9	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	9	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	9	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	9	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	17	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	17	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	17	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	17	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	17	0.26
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	17	0.26
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	3	0.26
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	3	0.26
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	15	0.26
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	15	0.26
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	17	0.26
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	17	0.26
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	1	0.26
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	1	0.26
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	1	0.26
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	12	0.26
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	12	0.26
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	12	0.26
(1,672)	1:97:A:ALA:HB1	1:98:A:ILE:HB	18	0.26
(1,672)	1:97:A:ALA:HB2	1:98:A:ILE:HB	18	0.26
(1,672)	1:97:A:ALA:HB3	1:98:A:ILE:HB	18	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	2	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	2	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	7	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	7	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	12	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	12	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	13	0.26
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	13	0.26
(1,594)	1:89:A:THR:HG23	1:90:A:PHE:HB2	15	0.26
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	3	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	3	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	3	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	3	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	3	0.26
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	6	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	6	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	6	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	6	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	6	0.26
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	6	0.26
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	7	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	7	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	7	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	7	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	7	0.26
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	7	0.26
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	8	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	8	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	8	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	8	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	8	0.26
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	8	0.26
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	11	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	11	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	11	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	11	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	11	0.26
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	11	0.26
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	13	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	13	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	13	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	13	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	13	0.26
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	13	0.26
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	19	0.26
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	19	0.26
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	19	0.26
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	19	0.26
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	19	0.26
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	19	0.26
(1,564)	1:87:A:LEU:HD23	1:60:A:ILE:HG21	5	0.26
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	17	0.26
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	17	0.26
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	17	0.26
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	17	0.26
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	17	0.26
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	17	0.26
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	17	0.26
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	17	0.26
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	17	0.26
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	17	0.26
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	17	0.26
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	9	0.26
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	9	0.26
(1,475)	1:79:A:ILE:HG21	1:78:A:LYS:HG2	18	0.26
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	14	0.26
(1,340)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	11	0.26
(1,311)	1:58:A:ILE:HG12	1:57:A:THR:HB	1	0.26
(1,311)	1:58:A:ILE:HG12	1:57:A:THR:HB	16	0.26
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	19	0.26
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	11	0.26
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	11	0.26
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	11	0.26
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	11	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	10	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	10	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	13	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	13	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	16	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	16	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	17	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	17	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	18	0.26
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	18	0.26
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	20	0.26
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	4	0.26
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	4	0.26
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	15	0.26
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	15	0.26
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	19	0.26
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	19	0.26
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	19	0.25
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	14	0.25
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	14	0.25
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	11	0.25
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	12	0.25
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	12	0.25
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	2	0.25
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	2	0.25
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	9	0.25
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	9	0.25
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	10	0.25
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	10	0.25
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	9	0.25
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	9	0.25
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	14	0.25
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	14	0.25
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	6	0.25
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	6	0.25
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	10	0.25
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	19	0.25
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	17	0.25
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	17	0.25
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB2	15	0.25
(1,2823)	1:88:A:SER:H	1:87:A:LEU:HB3	15	0.25
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	7	0.25
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	7	0.25
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	11	0.25
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	11	0.25
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	13	0.25
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	13	0.25
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	4	0.25
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	7	0.25
(1,2764)	1:103:B:THR:HG22	1:105:B:ILE:HB	8	0.25
(1,2764)	1:103:B:THR:HG23	1:105:B:ILE:HB	16	0.25
(1,2764)	1:103:B:THR:HG22	1:105:B:ILE:HB	20	0.25
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	8	0.25
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	8	0.25
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	8	0.25
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	4	0.25
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	4	0.25
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	4	0.25
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	4	0.25
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	4	0.25
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	4	0.25
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	4	0.25
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	4	0.25
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	4	0.25
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	4	0.25
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	4	0.25
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	4	0.25
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	4	0.25
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	4	0.25
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	4	0.25
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	4	0.25
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	4	0.25
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	4	0.25
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	4	0.25
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	4	0.25
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	4	0.25
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	4	0.25
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	4	0.25
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	4	0.25
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	4	0.25
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	4	0.25
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	4	0.25
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	4	0.25
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	4	0.25
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	4	0.25
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	4	0.25
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	4	0.25
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	4	0.25
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	4	0.25
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	4	0.25
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	5	0.25
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	19	0.25
(1,2376)	1:58:B:ILE:HG13	1:56:B:PRO:HB2	13	0.25
(1,2117)	1:103:B:THR:HG23	1:102:B:ILE:HB	17	0.25
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	6	0.25
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	12	0.25
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	18	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	3	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	3	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	3	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	3	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	3	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	3	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	9	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	9	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	9	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	9	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	9	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	20	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	20	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	20	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	20	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	20	0.25
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	20	0.25
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	2	0.25
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	2	0.25
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	4	0.25
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	4	0.25
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	9	0.25
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	9	0.25
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	12	0.25
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	12	0.25
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	12	0.25
(1,2053)	1:69:B:THR:HG21	1:98:B:ILE:H	14	0.25
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	4	0.25
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	4	0.25
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	12	0.25
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	12	0.25
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	15	0.25
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	15	0.25
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	2	0.25
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	2	0.25
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	2	0.25
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	2	0.25
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	2	0.25
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	2	0.25
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	18	0.25
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	18	0.25
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	18	0.25
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	18	0.25
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	18	0.25
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	18	0.25
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG21	4	0.25
(1,1948)	1:87:B:LEU:HD21	1:60:B:ILE:HG21	18	0.25
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	14	0.25
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	14	0.25
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	14	0.25
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	14	0.25
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	14	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	2	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	2	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	2	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	2	0.25
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	2	0.25
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	2	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	2	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	2	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	2	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	2	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	2	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	2	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	9	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	9	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	9	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	9	0.25
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	9	0.25
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	9	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	9	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	9	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	9	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	9	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	9	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	9	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	20	0.25
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	20	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	20	0.25
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	20	0.25
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	20	0.25
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	20	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	20	0.25
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	20	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	20	0.25
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	20	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	20	0.25
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	20	0.25
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG13	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	12	0.25
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	12	0.25
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	7	0.25
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	7	0.25
(1,1859)	1:79:B:ILE:HG23	1:78:B:LYS:HG2	7	0.25
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	4	0.25
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	4	0.25
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	4	0.25
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	4	0.25
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	4	0.25
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	4	0.25
(1,1801)	1:37:B:VAL:HG23	1:73:B:THR:HG1	20	0.25
(1,1793)	1:69:B:THR:HG1	1:54:B:LEU:HA	5	0.25
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD12	20	0.25
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	19	0.25
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	19	0.25
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	19	0.25
(1,1662)	1:48:B:LYS:HD3	1:43:B:ILE:HG21	18	0.25
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	5	0.25
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	1	0.25
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	1	0.25
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	14	0.25
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	14	0.25
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	18	0.25
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	18	0.25
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	15	0.25
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	15	0.25
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	1	0.25
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	1	0.25
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	15	0.25
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	15	0.25
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	19	0.25
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	19	0.25
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	20	0.25
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	20	0.25
(1,992)	1:58:A:ILE:HG21	1:56:A:PRO:HB2	11	0.25
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG2	7	0.25
(1,772)	1:10:A:LYS:HA	1:10:A:LYS:HG3	7	0.25
(1,733)	1:103:A:THR:HG22	1:102:A:ILE:HB	3	0.25
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	11	0.25
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	11	0.25
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	11	0.25
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	11	0.25
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	11	0.25
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	10	0.25
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	10	0.25
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	15	0.25
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	15	0.25
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	17	0.25
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	17	0.25
(1,643)	1:94:A:ILE:HG21	1:24:A:VAL:HG21	7	0.25
(1,594)	1:89:A:THR:HG23	1:90:A:PHE:HB2	4	0.25
(1,594)	1:89:A:THR:HG21	1:90:A:PHE:HB2	13	0.25
(1,575)	1:89:A:THR:HG21	1:87:A:LEU:HB2	7	0.25
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	1	0.25
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	1	0.25
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	1	0.25
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	1	0.25
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	1	0.25
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	1	0.25
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	10	0.25
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	10	0.25
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	10	0.25
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	10	0.25
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	10	0.25
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	10	0.25
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	12	0.25
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	12	0.25
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	12	0.25
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	12	0.25
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	12	0.25
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	12	0.25
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	14	0.25
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	14	0.25
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	14	0.25
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	14	0.25
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	14	0.25
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	14	0.25
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	16	0.25
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	16	0.25
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	16	0.25
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	16	0.25
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	16	0.25
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	17	0.25
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	17	0.25
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	17	0.25
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	17	0.25
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	17	0.25
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	17	0.25
(1,564)	1:87:A:LEU:HD13	1:60:A:ILE:HG21	20	0.25
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	17	0.25
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	17	0.25
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	17	0.25
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	17	0.25
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	17	0.25
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	17	0.25
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	8	0.25
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	8	0.25
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	8	0.25
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	8	0.25
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	8	0.25
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	8	0.25
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	8	0.25
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	8	0.25
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	8	0.25
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	8	0.25
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	8	0.25
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	8	0.25
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	15	0.25
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	15	0.25
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	15	0.25
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	15	0.25
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	15	0.25
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	15	0.25
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	15	0.25
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	15	0.25
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	15	0.25
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	15	0.25
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	15	0.25
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	15	0.25
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	4	0.25
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	4	0.25
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	8	0.25
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	16	0.25
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	16	0.25
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	16	0.25
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	16	0.25
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	16	0.25
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	16	0.25
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG22	7	0.25
(1,338)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	1	0.25
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	1	0.25
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	12	0.25
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	13	0.25
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	17	0.25
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	6	0.25
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	6	0.25
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	6	0.25
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	6	0.25
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	10	0.25
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	10	0.25
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	10	0.25
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	10	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	3	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	3	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	11	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	11	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	15	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	15	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	19	0.25
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	19	0.25
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	3	0.25
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	3	0.25
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	10	0.25
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	10	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	1	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	1	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	5	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	5	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	9	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	9	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	11	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	11	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	12	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	16	0.25
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	16	0.25
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	1	0.25
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	1	0.25
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	5	0.25
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	5	0.25
(1,54)	1:10:A:LYS:HD2	1:14:A:SER:HB2	5	0.25
(1,54)	1:10:A:LYS:HD2	1:14:A:SER:HB3	5	0.25
(1,54)	1:10:A:LYS:HD3	1:14:A:SER:HB2	5	0.25
(1,54)	1:10:A:LYS:HD3	1:14:A:SER:HB3	5	0.25
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	20	0.24
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	20	0.24
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	4	0.24
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	4	0.24
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	1	0.24
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	1	0.24
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	6	0.24
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	6	0.24
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	8	0.24
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	8	0.24
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	3	0.24
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	14	0.24
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	16	0.24
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	20	0.24
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	6	0.24
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	6	0.24
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	16	0.24
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	16	0.24
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	5	0.24
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	5	0.24
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD2	13	0.24
(1,2819)	1:82:A:GLU:H	1:10:A:LYS:HD3	13	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	1	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	1	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	6	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	6	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	12	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	12	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	15	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	15	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	16	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	19	0.24
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	19	0.24
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	1	0.24
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	1	0.24
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	12	0.24
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	18	0.24
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	18	0.24
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	3	0.24
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	14	0.24
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	8	0.24
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	8	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	1	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	1	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	2	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	2	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	3	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	3	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	4	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	4	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	5	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	5	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	6	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	6	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	7	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	7	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	8	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	8	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	9	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	9	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	10	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	10	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	11	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	11	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	12	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	12	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	13	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	13	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	14	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	14	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	16	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	16	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	17	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	18	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	18	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	19	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	19	0.24
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	20	0.24
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	20	0.24
(1,2117)	1:103:B:THR:HG21	1:102:B:ILE:HB	2	0.24
(1,2117)	1:103:B:THR:HG23	1:102:B:ILE:HB	15	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	16	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	16	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	16	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	16	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	16	0.24
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	16	0.24
(1,2073)	1:69:B:THR:HG23	1:100:B:PHE:HD2	5	0.24
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	3	0.24
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	3	0.24
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	6	0.24
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	6	0.24
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	8	0.24
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	8	0.24
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	15	0.24
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	15	0.24
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	16	0.24
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	16	0.24
(1,2056)	1:97:B:ALA:HB1	1:98:B:ILE:HB	4	0.24
(1,2056)	1:97:B:ALA:HB2	1:98:B:ILE:HB	4	0.24
(1,2056)	1:97:B:ALA:HB3	1:98:B:ILE:HB	4	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	2	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	2	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	14	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	14	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	17	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	17	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	19	0.24
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	19	0.24
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	8	0.24
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	8	0.24
(1,1978)	1:89:B:THR:HG21	1:90:B:PHE:HB2	1	0.24
(1,1978)	1:89:B:THR:HG23	1:90:B:PHE:HB2	9	0.24
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	5	0.24
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	5	0.24
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	5	0.24
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	5	0.24
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	5	0.24
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	6	0.24
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	6	0.24
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	6	0.24
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	6	0.24
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	6	0.24
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	6	0.24
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	9	0.24
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	9	0.24
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	9	0.24
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	9	0.24
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	9	0.24
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	9	0.24
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	16	0.24
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	16	0.24
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	16	0.24
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	16	0.24
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	16	0.24
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	16	0.24
(1,1948)	1:87:B:LEU:HD12	1:60:B:ILE:HG21	16	0.24
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	20	0.24
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	20	0.24
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	20	0.24
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	20	0.24
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	20	0.24
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	20	0.24
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	14	0.24
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	14	0.24
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	14	0.24
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	14	0.24
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	14	0.24
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	14	0.24
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	14	0.24
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	14	0.24
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	14	0.24
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	14	0.24
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	14	0.24
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	19	0.24
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	19	0.24
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	19	0.24
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	19	0.24
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	19	0.24
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	19	0.24
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	19	0.24
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	19	0.24
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	19	0.24
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	19	0.24
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	19	0.24
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	19	0.24
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	7	0.24
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	7	0.24
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	2	0.24
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	2	0.24
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	15	0.24
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	15	0.24
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	15	0.24
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	15	0.24
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	5	0.24
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	5	0.24
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	5	0.24
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	10	0.24
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	10	0.24
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	10	0.24
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	10	0.24
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	10	0.24
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	13	0.24
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	13	0.24
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	13	0.24
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	13	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	2	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	2	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	3	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	3	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	13	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	13	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	16	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	16	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	20	0.24
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	12	0.24
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	12	0.24
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	17	0.24
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	17	0.24
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	18	0.24
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	18	0.24
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	4	0.24
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	4	0.24
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	9	0.24
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	9	0.24
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	16	0.24
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	16	0.24
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	1	0.24
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	1	0.24
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	10	0.24
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	10	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	1	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	1	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	3	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	3	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	5	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	5	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	7	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	7	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	10	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	10	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	11	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	11	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	12	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	12	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	13	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	13	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	14	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	14	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	16	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	16	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	17	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	17	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	18	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	18	0.24
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	20	0.24
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	1	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	1	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	3	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	3	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	5	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	5	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	7	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	7	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	10	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	10	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	11	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	11	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	12	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	12	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	13	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	13	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	14	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	14	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	16	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	16	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	17	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	17	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	18	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	18	0.24
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	20	0.24
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	20	0.24
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	5	0.24
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	5	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	1	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	1	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	2	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	2	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	3	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	3	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	4	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	4	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	5	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	5	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	6	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	6	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	7	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	8	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	8	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	9	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	9	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	10	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	10	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	11	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	11	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	12	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	12	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	13	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	13	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	14	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	14	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	16	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	16	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	17	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	17	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	18	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	18	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	19	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	19	0.24
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	20	0.24
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	20	0.24
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	13	0.24
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	13	0.24
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	13	0.24
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	13	0.24
(1,1380)	1:103:A:THR:HG21	1:105:A:ILE:HB	8	0.24
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	17	0.24
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	17	0.24
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	17	0.24
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	1	0.24
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	1	0.24
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	1	0.24
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	1	0.24
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	1	0.24
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	1	0.24
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	1	0.24
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	1	0.24
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	1	0.24
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	1	0.24
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	1	0.24
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	1	0.24
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	1	0.24
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	1	0.24
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	1	0.24
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	1	0.24
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	1	0.24
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	1	0.24
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	1	0.24
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	1	0.24
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	1	0.24
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	1	0.24
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	1	0.24
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	1	0.24
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	1	0.24
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	1	0.24
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	1	0.24
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	1	0.24
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	1	0.24
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	1	0.24
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	1	0.24
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	1	0.24
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	1	0.24
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	1	0.24
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	1	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	1	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	1	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	2	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	2	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	3	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	3	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	4	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	4	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	5	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	5	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	6	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	6	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	7	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	7	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	8	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	9	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	9	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	10	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	10	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	11	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	11	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	12	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	12	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	13	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	13	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	14	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	14	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	15	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	15	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	16	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	16	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	17	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	17	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	18	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	18	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	19	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	19	0.24
(1,758)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	20	0.24
(1,758)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	20	0.24
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	13	0.24
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	10	0.24
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	10	0.24
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	10	0.24
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	10	0.24
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	10	0.24
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	10	0.24
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	7	0.24
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	7	0.24
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	9	0.24
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	9	0.24
(1,647)	1:93:A:GLU:HG2	1:94:A:ILE:HG12	3	0.24
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	4	0.24
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	4	0.24
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	14	0.24
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	14	0.24
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	20	0.24
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	4	0.24
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	4	0.24
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	17	0.24
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	17	0.24
(1,594)	1:89:A:THR:HG1	1:90:A:PHE:HB2	5	0.24
(1,594)	1:89:A:THR:HG22	1:90:A:PHE:HB2	6	0.24
(1,594)	1:89:A:THR:HG21	1:90:A:PHE:HB2	12	0.24
(1,581)	1:58:A:ILE:HG23	1:90:A:PHE:HD2	19	0.24
(1,575)	1:89:A:THR:HG21	1:87:A:LEU:HB2	14	0.24
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	15	0.24
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	15	0.24
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	15	0.24
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	15	0.24
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	15	0.24
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	15	0.24
(1,564)	1:87:A:LEU:HD23	1:60:A:ILE:HG21	8	0.24
(1,544)	1:85:A:ASN:HB3	1:60:A:ILE:HG23	12	0.24
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	11	0.24
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	15	0.24
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	15	0.24
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	15	0.24
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	15	0.24
(1,338)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	12	0.24
(1,332)	1:61:A:ASP:HB2	1:60:A:ILE:HG13	2	0.24
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	2	0.24
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	11	0.24
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	14	0.24
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	15	0.24
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	8	0.24
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	8	0.24
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	6	0.24
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	8	0.24
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	8	0.24
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	6	0.24
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	6	0.24
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	8	0.24
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	8	0.24
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	18	0.24
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	18	0.24
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	19	0.24
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	19	0.24
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	20	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	3	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	3	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	6	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	6	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	7	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	7	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	8	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	8	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	11	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	11	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	12	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	12	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	13	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	13	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	14	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	14	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	15	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	15	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	17	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	17	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	18	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	18	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	19	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	19	0.24
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	20	0.24
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	20	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	3	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	3	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	6	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	6	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	7	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	7	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	8	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	8	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	11	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	11	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	12	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	12	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	13	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	13	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	14	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	15	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	15	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	17	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	17	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	18	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	18	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	19	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	19	0.24
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	20	0.24
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	20	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	1	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	1	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	3	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	3	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	5	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	5	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	18	0.24
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	18	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	1	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	1	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	2	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	2	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	3	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	3	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	4	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	4	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	5	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	5	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	6	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	6	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	7	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	7	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	8	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	8	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	9	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	9	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	10	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	10	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	11	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	11	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	12	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	13	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	13	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	14	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	14	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	15	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	15	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	16	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	16	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	17	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	17	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	18	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	18	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	19	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	19	0.24
(1,32)	1:7:A:TYR:HB2	1:7:A:TYR:HB3	20	0.24
(1,32)	1:7:A:TYR:HB3	1:7:A:TYR:HB2	20	0.24
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	11	0.23
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	11	0.23
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	11	0.23
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	3	0.23
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	3	0.23
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	15	0.23
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	15	0.23
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	5	0.23
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	5	0.23
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	17	0.23
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	5	0.23
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	5	0.23
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	19	0.23
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	19	0.23
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	2	0.23
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	2	0.23
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	7	0.23
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	11	0.23
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	6	0.23
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	11	0.23
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	7	0.23
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	7	0.23
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	5	0.23
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	5	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	1	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	2	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	2	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	3	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	3	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	4	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	4	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	5	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	5	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	6	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	6	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	7	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	7	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	8	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	8	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	9	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	9	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	10	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	10	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	11	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	11	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	12	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	12	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	13	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	13	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	14	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	14	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	15	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	15	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	16	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	16	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	17	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	17	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	18	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	18	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	19	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	19	0.23
(1,2654)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	20	0.23
(1,2654)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	20	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	1	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	1	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	2	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	3	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	3	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	4	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	4	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	5	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	5	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	6	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	6	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	7	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	7	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	9	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	9	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	10	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	10	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	11	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	11	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	12	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	12	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	13	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	13	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	14	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	14	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	15	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	15	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	16	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	16	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	17	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	17	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	18	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	18	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	19	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	19	0.23
(1,2642)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	20	0.23
(1,2642)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	20	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	1	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	1	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	2	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	2	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	3	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	3	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	4	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	5	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	5	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	6	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	6	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	7	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	7	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	8	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	8	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	9	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	9	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	10	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	10	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	11	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	11	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	12	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	12	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	13	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	13	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	14	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	14	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	15	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	15	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	16	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	16	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	17	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	17	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	18	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	18	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	19	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	19	0.23
(1,2633)	1:88:B:SER:HB2	1:88:B:SER:HB3	20	0.23
(1,2633)	1:88:B:SER:HB3	1:88:B:SER:HB2	20	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	1	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	1	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	2	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	2	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	3	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	3	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	4	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	4	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	5	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	6	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	6	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	7	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	7	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	8	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	8	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	9	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	9	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	10	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	10	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	11	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	11	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	12	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	12	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	13	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	13	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	14	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	14	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	15	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	15	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	16	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	16	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	17	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	17	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	18	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	18	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	19	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	19	0.23
(1,2632)	1:88:B:SER:HB2	1:88:B:SER:HB3	20	0.23
(1,2632)	1:88:B:SER:HB3	1:88:B:SER:HB2	20	0.23
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	14	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	1	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	1	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	2	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	2	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	3	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	3	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	4	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	4	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	5	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	6	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	6	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	7	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	7	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	8	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	8	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	9	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	9	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	10	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	10	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	11	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	11	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	12	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	12	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	13	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	13	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	14	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	14	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	15	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	15	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	16	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	16	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	17	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	17	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	18	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	18	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	19	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	19	0.23
(1,2416)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	20	0.23
(1,2416)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	20	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	1	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	1	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	2	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	2	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	3	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	3	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	4	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	4	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	5	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	5	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	6	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	7	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	7	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	8	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	8	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	9	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	9	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	10	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	10	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	11	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	11	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	12	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	12	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	13	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	13	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	14	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	14	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	15	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	15	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	16	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	16	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	17	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	17	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	18	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	18	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	19	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	19	0.23
(1,2415)	1:64:B:ASP:HB2	1:64:B:ASP:HB3	20	0.23
(1,2415)	1:64:B:ASP:HB3	1:64:B:ASP:HB2	20	0.23
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	2	0.23
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	2	0.23
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	14	0.23
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	14	0.23
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	18	0.23
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	18	0.23
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	20	0.23
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	20	0.23
(1,2142)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	15	0.23
(1,2142)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	15	0.23
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	15	0.23
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG23	7	0.23
(1,2114)	1:103:B:THR:HG1	1:99:B:ASP:HB2	4	0.23
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	15	0.23
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	15	0.23
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	15	0.23
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	15	0.23
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	15	0.23
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	15	0.23
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	17	0.23
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	17	0.23
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	20	0.23
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	20	0.23
(1,2053)	1:69:B:THR:HG21	1:98:B:ILE:H	6	0.23
(1,2053)	1:69:B:THR:HG22	1:98:B:ILE:H	10	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	1	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	1	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	5	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	5	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	6	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	6	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	10	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	10	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	13	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	13	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	16	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	16	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	20	0.23
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	20	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	1	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	1	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	2	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	2	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	3	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	3	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	4	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	4	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	5	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	5	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	6	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	6	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	7	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	7	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	8	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	9	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	9	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	10	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	10	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	11	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	11	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	12	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	12	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	13	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	13	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	14	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	14	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	15	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	15	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	16	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	16	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	17	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	17	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	18	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	18	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	19	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	19	0.23
(1,1994)	1:91:B:ARG:HB2	1:91:B:ARG:HB3	20	0.23
(1,1994)	1:91:B:ARG:HB3	1:91:B:ARG:HB2	20	0.23
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	4	0.23
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	4	0.23
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	6	0.23
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	6	0.23
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	7	0.23
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	7	0.23
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	9	0.23
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	9	0.23
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	13	0.23
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	13	0.23
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	18	0.23
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	18	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	1	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	1	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	2	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	2	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	3	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	4	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	4	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	5	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	5	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	6	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	6	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	7	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	7	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	9	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	9	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	10	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	10	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	11	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	11	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	12	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	12	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	13	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	13	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	14	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	14	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	15	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	15	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	16	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	16	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	17	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	17	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	18	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	18	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	19	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	19	0.23
(1,1983)	1:90:B:PHE:HB2	1:90:B:PHE:HB3	20	0.23
(1,1983)	1:90:B:PHE:HB3	1:90:B:PHE:HB2	20	0.23
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	7	0.23
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	7	0.23
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	7	0.23
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	7	0.23
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	7	0.23
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	7	0.23
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	7	0.23
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	7	0.23
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	7	0.23
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	7	0.23
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	7	0.23
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	7	0.23
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	7	0.23
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	7	0.23
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	7	0.23
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	7	0.23
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	7	0.23
(1,1952)	1:87:B:LEU:HD11	1:87:B:LEU:HA	13	0.23
(1,1952)	1:87:B:LEU:HD12	1:87:B:LEU:HA	13	0.23
(1,1952)	1:87:B:LEU:HD13	1:87:B:LEU:HA	13	0.23
(1,1952)	1:87:B:LEU:HD21	1:87:B:LEU:HA	13	0.23
(1,1952)	1:87:B:LEU:HD22	1:87:B:LEU:HA	13	0.23
(1,1952)	1:87:B:LEU:HD23	1:87:B:LEU:HA	13	0.23
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG21	14	0.23
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	12	0.23
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	12	0.23
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	12	0.23
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	12	0.23
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	12	0.23
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	12	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	3	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	3	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	3	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	3	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	3	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	3	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	3	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	3	0.23
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	3	0.23
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	3	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	3	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	3	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	10	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	10	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	10	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	10	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	10	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	10	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	10	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	10	0.23
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	10	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	10	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	10	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	11	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	11	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	11	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	11	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	11	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	11	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	11	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	11	0.23
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	11	0.23
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	11	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	11	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	11	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	16	0.23
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	16	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	16	0.23
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	16	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	16	0.23
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	16	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	16	0.23
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	16	0.23
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	16	0.23
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	16	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	16	0.23
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	16	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	1	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	1	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	2	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	2	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	3	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	3	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	4	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	4	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	5	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	5	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	6	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	6	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	7	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	7	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	8	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	9	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	9	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	10	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	10	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	11	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	11	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	12	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	12	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	13	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	13	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	14	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	14	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	15	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	15	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	16	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	16	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	17	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	17	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	18	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	18	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	19	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	19	0.23
(1,1936)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	20	0.23
(1,1936)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	20	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	1	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	1	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	2	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	2	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	3	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	3	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	4	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	4	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	5	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	5	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	6	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	6	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	7	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	7	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	8	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	8	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	9	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	10	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	10	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	11	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	11	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	12	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	12	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	13	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	13	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	14	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	14	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	15	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	15	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	16	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	16	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	17	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	17	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	18	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	18	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	19	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	19	0.23
(1,1935)	1:85:B:ASN:HB2	1:85:B:ASN:HB3	20	0.23
(1,1935)	1:85:B:ASN:HB3	1:85:B:ASN:HB2	20	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	6	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	6	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	6	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	6	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	6	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	6	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	6	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	6	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	6	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	6	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	6	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	6	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	15	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	15	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	15	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	15	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	15	0.23
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	15	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	15	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	15	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	15	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	15	0.23
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	15	0.23
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	6	0.23
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	6	0.23
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	11	0.23
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	11	0.23
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	11	0.23
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	11	0.23
(1,1804)	1:73:B:THR:HG23	1:39:B:PRO:HG3	19	0.23
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	9	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	1	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	1	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	2	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	2	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	3	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	3	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	4	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	4	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	5	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	5	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	6	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	6	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	7	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	7	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	8	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	8	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	9	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	9	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	10	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	10	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	11	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	11	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	13	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	13	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	17	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	17	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	18	0.23
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	18	0.23
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	19	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	1	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	1	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	2	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	2	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	3	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	3	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	4	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	4	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	5	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	5	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	6	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	6	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	7	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	7	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	8	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	8	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	9	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	9	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	10	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	10	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	11	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	11	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	13	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	13	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	17	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	17	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	18	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	18	0.23
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	19	0.23
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	19	0.23
(1,1725)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	10	0.23
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	6	0.23
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	6	0.23
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	6	0.23
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	8	0.23
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	8	0.23
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	8	0.23
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	10	0.23
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	10	0.23
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	10	0.23
(1,1695)	1:58:B:ILE:HG12	1:57:B:THR:HB	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG13	13	0.23
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	4	0.23
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	4	0.23
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	11	0.23
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	11	0.23
(1,1662)	1:48:B:LYS:HD3	1:43:B:ILE:HG21	9	0.23
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	3	0.23
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	4	0.23
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	9	0.23
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	17	0.23
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	17	0.23
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	17	0.23
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	17	0.23
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	11	0.23
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	11	0.23
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	20	0.23
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	5	0.23
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	5	0.23
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB2	6	0.23
(1,1544)	1:28:B:LEU:HA	1:26:B:SER:HB3	6	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	1	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	1	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	2	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	2	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	3	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	3	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	4	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	4	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	5	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	5	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	6	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	6	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	7	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	7	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	8	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	8	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	9	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	9	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	10	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	10	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	11	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	12	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	12	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	13	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	13	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	14	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	14	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	15	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	15	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	16	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	16	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	17	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	17	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	18	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	18	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	19	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	19	0.23
(1,1543)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	20	0.23
(1,1543)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	20	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	1	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	1	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	2	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	2	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	3	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	3	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	4	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	4	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	5	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	5	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	6	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	6	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	7	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	7	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	8	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	8	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	9	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	9	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	10	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	10	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	11	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	11	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	12	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	13	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	13	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	14	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	14	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	15	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	15	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	16	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	16	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	17	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	17	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	18	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	18	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	19	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	19	0.23
(1,1542)	1:27:B:ASP:HB2	1:27:B:ASP:HB3	20	0.23
(1,1542)	1:27:B:ASP:HB3	1:27:B:ASP:HB2	20	0.23
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	2	0.23
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	2	0.23
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	14	0.23
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	14	0.23
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	18	0.23
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	18	0.23
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	20	0.23
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	20	0.23
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	15	0.23
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	15	0.23
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	2	0.23
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	2	0.23
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	4	0.23
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	4	0.23
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	6	0.23
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	6	0.23
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	8	0.23
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	8	0.23
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	9	0.23
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	9	0.23
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	15	0.23
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	15	0.23
(1,1488)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	19	0.23
(1,1488)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	19	0.23
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	2	0.23
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	4	0.23
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	4	0.23
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	6	0.23
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	6	0.23
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	8	0.23
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	8	0.23
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	9	0.23
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	9	0.23
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	15	0.23
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	15	0.23
(1,1487)	1:21:B:PHE:HB2	1:21:B:PHE:HB3	19	0.23
(1,1487)	1:21:B:PHE:HB3	1:21:B:PHE:HB2	19	0.23
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	1	0.23
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	1	0.23
(1,1416)	1:7:B:TYR:HB2	1:7:B:TYR:HB3	15	0.23
(1,1416)	1:7:B:TYR:HB3	1:7:B:TYR:HB2	15	0.23
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG21	19	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	1	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	1	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	2	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	2	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	3	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	3	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	4	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	4	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	5	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	5	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	6	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	6	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	7	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	7	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	8	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	8	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	9	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	9	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	10	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	10	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	11	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	11	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	12	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	12	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	14	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	15	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	15	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	16	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	16	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	17	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	17	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	18	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	18	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	19	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	19	0.23
(1,1395)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	20	0.23
(1,1395)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	20	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	1	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	1	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	2	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	2	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	3	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	3	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	4	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	4	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	5	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	5	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	6	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	6	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	7	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	7	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	8	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	8	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	9	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	9	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	10	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	10	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	11	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	11	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	12	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	12	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	14	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	14	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	15	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	15	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	16	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	17	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	17	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	18	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	18	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	19	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	19	0.23
(1,1394)	1:4:B:PHE:HB2	1:4:B:PHE:HB3	20	0.23
(1,1394)	1:4:B:PHE:HB3	1:4:B:PHE:HB2	20	0.23
(1,1376)	1:103:A:THR:HG21	1:103:A:THR:HA	1	0.23
(1,1287)	1:90:A:PHE:HB3	1:94:A:ILE:HG12	1	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	1	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	1	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	2	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	2	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	3	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	3	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	4	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	4	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	5	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	5	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	6	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	6	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	7	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	7	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	8	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	8	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	9	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	9	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	10	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	10	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	11	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	11	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	12	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	12	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	13	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	13	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	14	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	14	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	15	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	15	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	16	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	17	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	17	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	18	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	18	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	19	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	19	0.23
(1,1270)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	20	0.23
(1,1270)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	20	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	1	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	1	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	2	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	2	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	3	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	3	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	4	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	4	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	5	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	5	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	6	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	6	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	7	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	7	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	8	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	8	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	9	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	9	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	10	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	10	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	11	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	11	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	12	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	12	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	13	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	13	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	14	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	14	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	15	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	15	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	16	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	16	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	18	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	19	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	19	0.23
(1,1258)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	20	0.23
(1,1258)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	20	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	1	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	1	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	2	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	2	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	3	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	3	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	4	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	4	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	5	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	5	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	6	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	6	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	7	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	7	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	8	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	8	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	9	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	9	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	10	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	10	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	11	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	11	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	12	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	12	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	13	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	13	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	14	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	14	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	15	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	15	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	16	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	16	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	17	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	17	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	18	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	18	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	19	0.23
(1,1249)	1:88:A:SER:HB2	1:88:A:SER:HB3	20	0.23
(1,1249)	1:88:A:SER:HB3	1:88:A:SER:HB2	20	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	1	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	1	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	2	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	2	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	3	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	3	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	4	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	4	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	5	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	5	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	6	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	6	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	7	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	7	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	8	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	8	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	9	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	9	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	10	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	10	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	11	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	11	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	12	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	12	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	13	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	13	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	14	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	14	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	15	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	15	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	16	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	16	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	17	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	17	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	18	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	18	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	19	0.23
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	19	0.23
(1,1248)	1:88:A:SER:HB2	1:88:A:SER:HB3	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:88:A:SER:HB3	1:88:A:SER:HB2	20	0.23
(1,1048)	1:41:A:THR:HG22	1:66:A:ILE:HB	19	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	1	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	1	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	2	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	2	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	3	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	3	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	4	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	4	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	5	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	5	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	6	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	6	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	7	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	7	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	8	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	8	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	9	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	9	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	10	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	10	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	11	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	11	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	12	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	12	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	13	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	13	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	14	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	14	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	15	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	15	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	16	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	16	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	17	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	17	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	18	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	18	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	19	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	19	0.23
(1,1032)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	20	0.23
(1,1032)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	1	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	1	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	2	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	2	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	3	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	3	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	4	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	4	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	5	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	5	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	6	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	6	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	7	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	7	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	8	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	8	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	9	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	9	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	10	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	10	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	11	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	11	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	12	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	12	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	13	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	13	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	14	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	14	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	15	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	15	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	16	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	16	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	17	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	17	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	18	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	18	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	19	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	19	0.23
(1,1031)	1:64:A:ASP:HB2	1:64:A:ASP:HB3	20	0.23
(1,1031)	1:64:A:ASP:HB3	1:64:A:ASP:HB2	20	0.23
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	13	0.23
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	13	0.23
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	13	0.23
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	2	0.23
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	2	0.23
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	3	0.23
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	3	0.23
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	15	0.23
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	15	0.23
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	17	0.23
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	17	0.23
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	20	0.23
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	20	0.23
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	19	0.23
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	19	0.23
(1,733)	1:103:A:THR:HG23	1:102:A:ILE:HB	17	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	5	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	5	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	5	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	5	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	5	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	5	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	7	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	7	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	7	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	7	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	7	0.23
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	7	0.23
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	1	0.23
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	1	0.23
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	4	0.23
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	4	0.23
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	5	0.23
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	5	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	1	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	1	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	5	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	5	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	18	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	18	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	19	0.23
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	19	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	1	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	2	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	2	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	3	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	3	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	4	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	4	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	5	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	5	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	6	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	6	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	7	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	7	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	8	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	8	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	9	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	9	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	10	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	10	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	11	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	11	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	12	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	12	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	13	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	13	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	14	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	14	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	15	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	15	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	16	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	16	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	17	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	17	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	18	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	18	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	19	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	19	0.23
(1,610)	1:91:A:ARG:HB2	1:91:A:ARG:HB3	20	0.23
(1,610)	1:91:A:ARG:HB3	1:91:A:ARG:HB2	20	0.23
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	1	0.23
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	1	0.23
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	7	0.23
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	12	0.23
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	12	0.23
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	17	0.23
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	17	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	1	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	1	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	2	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	2	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	3	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	3	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	4	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	4	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	5	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	5	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	6	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	6	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	7	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	7	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	8	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	8	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	9	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	9	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	10	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	10	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	11	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	11	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	12	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	12	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	13	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	13	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	14	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	14	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	15	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	15	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	16	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	16	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	18	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	18	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	19	0.23
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	19	0.23
(1,599)	1:90:A:PHE:HB2	1:90:A:PHE:HB3	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:90:A:PHE:HB3	1:90:A:PHE:HB2	20	0.23
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	14	0.23
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	14	0.23
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	14	0.23
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	14	0.23
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	14	0.23
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	14	0.23
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	14	0.23
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	14	0.23
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	14	0.23
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	14	0.23
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	14	0.23
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	14	0.23
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	18	0.23
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	18	0.23
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	18	0.23
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	18	0.23
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	18	0.23
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	18	0.23
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	20	0.23
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	20	0.23
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	20	0.23
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	20	0.23
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	20	0.23
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	20	0.23
(1,564)	1:87:A:LEU:HD12	1:60:A:ILE:HG21	4	0.23
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	8	0.23
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	8	0.23
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	8	0.23
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	8	0.23
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	8	0.23
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	8	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	1	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	1	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	1	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	1	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	1	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	1	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	1	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	1	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	1	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	1	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	1	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	3	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	3	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	3	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	3	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	3	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	3	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	3	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	3	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	3	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	3	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	3	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	3	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	6	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	6	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	6	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	6	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	6	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	6	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	6	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	6	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	6	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	6	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	6	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	6	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	10	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	10	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	10	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	10	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	10	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	10	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	10	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	10	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	10	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	10	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	10	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	10	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	18	0.23
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	18	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	18	0.23
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	18	0.23
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	18	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	18	0.23
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	18	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	18	0.23
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	18	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	18	0.23
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	18	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	1	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	1	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	2	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	2	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	3	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	3	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	4	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	4	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	5	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	5	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	6	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	6	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	7	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	7	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	8	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	8	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	9	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	9	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	10	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	10	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	11	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	11	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	12	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	12	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	13	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	13	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	14	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	14	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	15	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	15	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	16	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	16	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	17	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	18	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	18	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	19	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	19	0.23
(1,552)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	20	0.23
(1,552)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	20	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	1	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	1	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	2	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	2	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	3	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	3	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	4	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	4	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	5	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	5	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	6	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	6	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	7	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	7	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	8	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	8	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	9	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	9	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	10	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	10	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	11	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	11	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	12	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	12	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	13	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	13	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	14	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	14	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	15	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	15	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	16	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	16	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	17	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	17	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	18	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	19	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	19	0.23
(1,551)	1:85:A:ASN:HB2	1:85:A:ASN:HB3	20	0.23
(1,551)	1:85:A:ASN:HB3	1:85:A:ASN:HB2	20	0.23
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	10	0.23
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	10	0.23
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	2	0.23
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	2	0.23
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	2	0.23
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	2	0.23
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	2	0.23
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	2	0.23
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	14	0.23
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	14	0.23
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	14	0.23
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	14	0.23
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	14	0.23
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	14	0.23
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	14	0.23
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG1	15	0.23
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	19	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	1	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	1	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	2	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	2	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	3	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	3	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	4	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	4	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	5	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	5	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	6	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	6	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	7	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	7	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	8	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	8	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	9	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	9	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	10	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	10	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	11	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	12	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	12	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	13	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	13	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	14	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	14	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	16	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	16	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	17	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	17	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	18	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	18	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	19	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	19	0.23
(1,376)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	20	0.23
(1,376)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	20	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	1	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	1	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	2	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	2	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	3	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	3	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	4	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	4	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	5	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	5	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	6	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	6	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	7	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	7	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	8	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	8	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	9	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	9	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	10	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	10	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	11	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	11	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	12	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	12	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	13	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	14	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	14	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	16	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	16	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	17	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	17	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	18	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	18	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	19	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	19	0.23
(1,375)	1:65:A:PHE:HB2	1:65:A:PHE:HB3	20	0.23
(1,375)	1:65:A:PHE:HB3	1:65:A:PHE:HB2	20	0.23
(1,363)	1:43:A:ILE:HG13	1:65:A:PHE:HD1	15	0.23
(1,342)	1:57:A:THR:HG23	1:64:A:ASP:HB3	7	0.23
(1,341)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	4	0.23
(1,340)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	7	0.23
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD12	7	0.23
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	10	0.23
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	10	0.23
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	10	0.23
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	12	0.23
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	12	0.23
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	12	0.23
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	15	0.23
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	15	0.23
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	15	0.23
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	16	0.23
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	16	0.23
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	16	0.23
(1,311)	1:58:A:ILE:HG12	1:57:A:THR:HB	11	0.23
(1,306)	1:56:A:PRO:HB2	1:58:A:ILE:HG21	11	0.23
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	8	0.23
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	8	0.23
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	14	0.23
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	14	0.23
(1,278)	1:48:A:LYS:HD2	1:43:A:ILE:HG21	7	0.23
(1,278)	1:48:A:LYS:HD3	1:43:A:ILE:HG21	16	0.23
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	20	0.23
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	2	0.23
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	2	0.23
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	14	0.23
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG22	9	0.23
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	9	0.23
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	9	0.23
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	17	0.23
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	17	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	1	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	1	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	2	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	2	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	3	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	3	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	4	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	4	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	5	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	5	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	6	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	6	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	7	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	7	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	8	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	8	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	9	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	9	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	10	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	10	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	11	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	11	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	12	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	12	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	13	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	13	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	14	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	14	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	15	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	15	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	16	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	16	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	17	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	17	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	18	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	19	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	19	0.23
(1,159)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	20	0.23
(1,159)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	20	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	1	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	1	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	2	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	2	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	3	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	3	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	4	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	4	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	5	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	5	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	6	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	6	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	7	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	7	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	8	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	8	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	9	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	9	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	10	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	10	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	11	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	11	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	12	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	12	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	13	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	13	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	14	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	14	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	15	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	15	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	16	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	16	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	17	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	17	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	18	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	18	0.23
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	19	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:27:A:ASP:HB2	1:27:A:ASP:HB3	20	0.23
(1,158)	1:27:A:ASP:HB3	1:27:A:ASP:HB2	20	0.23
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	2	0.23
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	2	0.23
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	3	0.23
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	3	0.23
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	15	0.23
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	15	0.23
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	17	0.23
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	17	0.23
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	20	0.23
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	20	0.23
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	6	0.23
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	6	0.23
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	1	0.23
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	1	0.23
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	2	0.23
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	2	0.23
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	4	0.23
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	4	0.23
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	5	0.23
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	5	0.23
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	9	0.23
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	9	0.23
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	10	0.23
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	10	0.23
(1,104)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	16	0.23
(1,104)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	16	0.23
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	1	0.23
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	1	0.23
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	2	0.23
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	2	0.23
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	4	0.23
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	4	0.23
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	5	0.23
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	5	0.23
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	9	0.23
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	9	0.23
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	10	0.23
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	10	0.23
(1,103)	1:21:A:PHE:HB2	1:21:A:PHE:HB3	16	0.23
(1,103)	1:21:A:PHE:HB3	1:21:A:PHE:HB2	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD1	20	0.23
(1,88)	1:7:A:TYR:HA	1:20:A:TYR:HD2	20	0.23
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	5	0.23
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	5	0.23
(1,66)	1:17:A:THR:HG1	1:16:A:LYS:HB3	8	0.23
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	19	0.23
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	19	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	1	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	1	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	2	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	2	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	3	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	3	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	4	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	4	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	5	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	5	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	6	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	6	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	7	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	7	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	8	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	8	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	9	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	9	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	10	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	10	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	11	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	11	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	12	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	12	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	13	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	13	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	14	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	14	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	15	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	15	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	16	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	16	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	17	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	17	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	18	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	19	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	19	0.23
(1,11)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	20	0.23
(1,11)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	20	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	1	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	1	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	2	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	2	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	3	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	3	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	4	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	4	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	5	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	5	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	6	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	6	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	7	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	7	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	8	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	8	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	9	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	9	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	10	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	10	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	11	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	11	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	12	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	12	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	13	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	13	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	14	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	14	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	15	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	15	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	16	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	16	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	17	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	17	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	18	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	18	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	19	0.23
(1,10)	1:4:A:PHE:HB2	1:4:A:PHE:HB3	20	0.23
(1,10)	1:4:A:PHE:HB3	1:4:A:PHE:HB2	20	0.23
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	15	0.22
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	17	0.22
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	17	0.22
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	18	0.22
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	18	0.22
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	1	0.22
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	1	0.22
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	20	0.22
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	20	0.22
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	18	0.22
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	15	0.22
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	15	0.22
(1,3061)	1:60:B:ILE:H	1:58:B:ILE:HG21	15	0.22
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	7	0.22
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	8	0.22
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	8	0.22
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	4	0.22
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	15	0.22
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	4	0.22
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	2	0.22
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	2	0.22
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	9	0.22
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	9	0.22
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	17	0.22
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	17	0.22
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	10	0.22
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	10	0.22
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	15	0.22
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	11	0.22
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	20	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	1	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	1	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	2	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	2	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	3	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	3	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	4	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	4	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	5	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	6	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	6	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	7	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	7	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	8	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	8	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	9	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	9	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	10	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	10	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	11	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	11	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	12	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	12	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	13	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	13	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	14	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	14	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	15	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	15	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	16	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	16	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	17	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	17	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	18	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	18	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	19	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	19	0.22
(1,2581)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	20	0.22
(1,2581)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	20	0.22
(1,2432)	1:41:B:THR:HG22	1:66:B:ILE:HB	11	0.22
(1,2432)	1:41:B:THR:HG22	1:66:B:ILE:HB	12	0.22
(1,2373)	1:57:B:THR:HG23	1:43:B:ILE:HG21	20	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	1	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	1	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	2	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	2	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	3	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	3	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	4	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	5	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	5	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	6	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	6	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	7	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	7	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	8	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	8	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	9	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	9	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	10	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	10	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	11	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	11	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	12	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	12	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	13	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	13	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	14	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	14	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	15	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	15	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	16	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	16	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	17	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	17	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	18	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	18	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	19	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	19	0.22
(1,2367)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	20	0.22
(1,2367)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	20	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	1	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	1	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	2	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	2	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	3	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	3	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	4	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	4	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	5	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	6	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	6	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	7	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	7	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	8	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	8	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	9	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	9	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	10	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	10	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	11	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	11	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	12	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	12	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	13	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	13	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	14	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	14	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	15	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	15	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	16	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	16	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	17	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	17	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	18	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	18	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	19	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	19	0.22
(1,2366)	1:56:B:PRO:HD2	1:56:B:PRO:HD3	20	0.22
(1,2366)	1:56:B:PRO:HD3	1:56:B:PRO:HD2	20	0.22
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB2	2	0.22
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB3	2	0.22
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB2	2	0.22
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB3	2	0.22
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB2	13	0.22
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB3	13	0.22
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB2	13	0.22
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB3	13	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	1	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	1	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	3	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	4	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	4	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	5	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	5	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	6	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	6	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	7	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	7	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	8	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	8	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	9	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	9	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	10	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	10	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	11	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	11	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	12	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	12	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	13	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	13	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	15	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	15	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	16	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	16	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	17	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	17	0.22
(1,2235)	1:26:B:SER:HB2	1:26:B:SER:HB3	19	0.22
(1,2235)	1:26:B:SER:HB3	1:26:B:SER:HB2	19	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	1	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	1	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	2	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	2	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	3	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	3	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	4	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	4	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	5	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	5	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	6	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	6	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	7	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	8	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	8	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	9	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	9	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	10	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	10	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	11	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	11	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	12	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	12	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	13	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	13	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	14	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	14	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	15	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	15	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	16	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	16	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	17	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	17	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	18	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	18	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	19	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	19	0.22
(1,2174)	1:14:B:SER:HB2	1:14:B:SER:HB3	20	0.22
(1,2174)	1:14:B:SER:HB3	1:14:B:SER:HB2	20	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	1	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	1	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	2	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	2	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	3	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	3	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	4	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	4	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	5	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	5	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	6	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	6	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	7	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	7	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	8	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	9	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	9	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	10	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	10	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	11	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	11	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	12	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	12	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	13	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	13	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	14	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	14	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	15	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	15	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	16	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	16	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	17	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	17	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	18	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	18	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	19	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	19	0.22
(1,2173)	1:14:B:SER:HB2	1:14:B:SER:HB3	20	0.22
(1,2173)	1:14:B:SER:HB3	1:14:B:SER:HB2	20	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	1	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	1	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	2	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	2	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	3	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	3	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	4	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	4	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	5	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	5	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	6	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	6	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	7	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	7	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	8	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	8	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	9	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	10	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	10	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	11	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	11	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	12	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	12	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	13	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	13	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	14	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	14	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	15	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	15	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	16	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	16	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	17	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	17	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	18	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	18	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	19	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	19	0.22
(1,2163)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	20	0.22
(1,2163)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	20	0.22
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG22	12	0.22
(1,2110)	1:101:B:LEU:HB3	1:102:B:ILE:HG13	4	0.22
(1,2085)	1:69:B:THR:HG23	1:101:B:LEU:HB3	19	0.22
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	7	0.22
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	7	0.22
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	10	0.22
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	10	0.22
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	12	0.22
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	12	0.22
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	18	0.22
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	18	0.22
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	7	0.22
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	7	0.22
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB2	11	0.22
(1,2030)	1:94:B:ILE:HA	1:93:B:GLU:HB3	11	0.22
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	1	0.22
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	1	0.22
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	2	0.22
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	2	0.22
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	3	0.22
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	10	0.22
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	10	0.22
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	15	0.22
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	15	0.22
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	17	0.22
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	17	0.22
(1,1978)	1:89:B:THR:HG21	1:90:B:PHE:HB2	4	0.22
(1,1978)	1:89:B:THR:HG23	1:90:B:PHE:HB2	5	0.22
(1,1978)	1:89:B:THR:HG22	1:90:B:PHE:HB2	19	0.22
(1,1948)	1:87:B:LEU:HD23	1:60:B:ILE:HG21	1	0.22
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	8	0.22
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	8	0.22
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	8	0.22
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	8	0.22
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	8	0.22
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	8	0.22
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	8	0.22
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	8	0.22
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	8	0.22
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	8	0.22
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	8	0.22
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	8	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	1	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	1	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	2	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	2	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	3	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	3	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	4	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	4	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	5	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	5	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	6	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	6	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	7	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	7	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	8	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	8	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	9	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	9	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	10	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	11	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	11	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	12	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	12	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	13	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	13	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	14	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	14	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	15	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	15	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	16	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	16	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	17	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	17	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	18	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	18	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	19	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	19	0.22
(1,1903)	1:83:B:PRO:HD2	1:83:B:PRO:HD3	20	0.22
(1,1903)	1:83:B:PRO:HD3	1:83:B:PRO:HD2	20	0.22
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	20	0.22
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	20	0.22
(1,1804)	1:73:B:THR:HG22	1:39:B:PRO:HG3	16	0.22
(1,1793)	1:69:B:THR:HG1	1:54:B:LEU:HA	9	0.22
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	19	0.22
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD12	11	0.22
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	12	0.22
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	12	0.22
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	14	0.22
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	14	0.22
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	16	0.22
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	16	0.22
(1,1760)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	20	0.22
(1,1760)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	20	0.22
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	12	0.22
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	12	0.22
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	14	0.22
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	14	0.22
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	16	0.22
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	16	0.22
(1,1759)	1:65:B:PHE:HB2	1:65:B:PHE:HB3	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1759)	1:65:B:PHE:HB3	1:65:B:PHE:HB2	20	0.22
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	9	0.22
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	9	0.22
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	9	0.22
(1,1696)	1:58:B:ILE:HG13	1:57:B:THR:HB	16	0.22
(1,1695)	1:58:B:ILE:HG13	1:57:B:THR:HB	16	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	5	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	5	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	10	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	10	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	12	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	12	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	14	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	14	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	15	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	15	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	16	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	16	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	18	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	18	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	20	0.22
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	20	0.22
(1,1649)	1:44:B:GLU:HA	1:43:B:ILE:HG13	15	0.22
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	4	0.22
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	4	0.22
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	3	0.22
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	7	0.22
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	2	0.22
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	6	0.22
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	16	0.22
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	16	0.22
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	19	0.22
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	19	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	1	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	1	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	3	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	3	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	4	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	4	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	5	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	5	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	6	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	7	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	7	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	8	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	8	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	9	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	9	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	10	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	10	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	11	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	11	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	12	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	12	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	13	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	13	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	15	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	15	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	16	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	16	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	17	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	17	0.22
(1,1540)	1:26:B:SER:HB2	1:26:B:SER:HB3	19	0.22
(1,1540)	1:26:B:SER:HB3	1:26:B:SER:HB2	19	0.22
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	4	0.22
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	4	0.22
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB2	9	0.22
(1,1499)	1:22:B:VAL:HB	1:21:B:PHE:HB3	9	0.22
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	9	0.22
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	9	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	1	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	1	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	2	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	2	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	3	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	3	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	4	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	4	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	5	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	5	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	6	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	6	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	7	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	8	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	8	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	9	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	9	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	10	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	10	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	11	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	11	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	12	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	12	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	13	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	13	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	14	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	14	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	15	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	15	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	16	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	16	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	17	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	17	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	18	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	18	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	19	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	19	0.22
(1,1435)	1:11:B:ASP:HB2	1:11:B:ASP:HB3	20	0.22
(1,1435)	1:11:B:ASP:HB3	1:11:B:ASP:HB2	20	0.22
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	1	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	1	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	1	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	2	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	2	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	3	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	3	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	4	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	4	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	5	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	5	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	6	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	6	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	7	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	8	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	8	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	9	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	9	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	10	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	10	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	11	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	11	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	12	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	12	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	13	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	13	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	14	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	14	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	15	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	15	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	16	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	16	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	17	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	17	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	18	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	18	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	19	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	19	0.22
(1,1197)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	20	0.22
(1,1197)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	20	0.22
(1,1157)	1:79:A:ILE:HD11	1:75:A:VAL:HB	13	0.22
(1,1157)	1:79:A:ILE:HD12	1:75:A:VAL:HB	13	0.22
(1,1157)	1:79:A:ILE:HD13	1:75:A:VAL:HB	13	0.22
(1,1029)	1:43:A:ILE:HG13	1:64:A:ASP:HB3	20	0.22
(1,997)	1:58:A:ILE:HA	1:58:A:ILE:HG13	19	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	1	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	1	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	2	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	2	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	3	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	3	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	4	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	4	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	5	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	5	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	6	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	7	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	7	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	8	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	8	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	9	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	9	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	10	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	10	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	11	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	11	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	12	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	12	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	14	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	14	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	15	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	15	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	17	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	17	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	18	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	18	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	19	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	19	0.22
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	20	0.22
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	20	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	1	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	1	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	2	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	2	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	3	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	3	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	4	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	4	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	5	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	5	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	6	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	6	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	7	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	7	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	8	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	8	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	9	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	10	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	10	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	11	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	11	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	12	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	12	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	14	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	14	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	15	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	15	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	17	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	17	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	18	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	18	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	19	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	19	0.22
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	20	0.22
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	20	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	1	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	1	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	4	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	4	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	5	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	5	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	6	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	6	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	7	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	7	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	8	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	8	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	9	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	9	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	10	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	10	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	11	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	11	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	12	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	12	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	13	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	13	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	14	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	16	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	16	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	18	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	18	0.22
(1,851)	1:26:A:SER:HB2	1:26:A:SER:HB3	19	0.22
(1,851)	1:26:A:SER:HB3	1:26:A:SER:HB2	19	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	2	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	2	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	3	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	3	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	4	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	4	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	5	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	5	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	6	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	6	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	7	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	7	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	8	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	8	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	9	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	9	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	10	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	10	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	11	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	11	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	12	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	12	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	13	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	13	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	14	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	14	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	15	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	15	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	16	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	16	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	17	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	17	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	18	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	18	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	19	0.22
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	20	0.22
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	20	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	2	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	2	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	3	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	3	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	4	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	4	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	5	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	5	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	6	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	6	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	7	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	7	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	8	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	8	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	9	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	9	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	10	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	10	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	11	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	11	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	12	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	12	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	13	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	13	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	14	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	14	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	15	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	15	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	16	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	16	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	17	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	17	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	18	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	18	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	19	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	19	0.22
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	20	0.22
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	20	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	1	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	2	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	2	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	3	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	3	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	4	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	4	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	5	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	5	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	6	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	6	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	7	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	7	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	8	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	8	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	9	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	9	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	10	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	10	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	11	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	11	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	12	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	12	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	13	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	13	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	14	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	14	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	15	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	15	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	16	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	16	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	17	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	17	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	18	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	18	0.22
(1,779)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	20	0.22
(1,779)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	20	0.22
(1,730)	1:103:A:THR:HG22	1:99:A:ASP:HB3	20	0.22
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	8	0.22
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	8	0.22
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	8	0.22
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	8	0.22
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	8	0.22
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	12	0.22
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	12	0.22
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	14	0.22
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	14	0.22
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	18	0.22
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	18	0.22
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	6	0.22
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	6	0.22
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	8	0.22
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	8	0.22
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	16	0.22
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	16	0.22
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	6	0.22
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	6	0.22
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	10	0.22
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	10	0.22
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	13	0.22
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	13	0.22
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	15	0.22
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	15	0.22
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	20	0.22
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	20	0.22
(1,581)	1:58:A:ILE:HG22	1:90:A:PHE:HD2	13	0.22
(1,564)	1:87:A:LEU:HD21	1:60:A:ILE:HG21	3	0.22
(1,564)	1:87:A:LEU:HD23	1:60:A:ILE:HG21	9	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	2	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	2	0.22
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	2	0.22
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	2	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	2	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	2	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	2	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	2	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	2	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	2	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	2	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	2	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	4	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	4	0.22
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	4	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	4	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	4	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	4	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	4	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	4	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	4	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	4	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	4	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	11	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	11	0.22
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	11	0.22
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	11	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	11	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	11	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	11	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	11	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	11	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	11	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	11	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	11	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	19	0.22
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	19	0.22
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	19	0.22
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	19	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	19	0.22
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	19	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	19	0.22
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	19	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	19	0.22
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	19	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	19	0.22
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	19	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	1	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	1	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	2	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	2	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	3	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	3	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	4	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	4	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	5	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	6	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	6	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	7	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	7	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	8	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	8	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	9	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	9	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	10	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	10	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	11	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	11	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	12	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	12	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	13	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	13	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	14	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	14	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	15	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	15	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	16	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	16	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	17	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	17	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	18	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	18	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	19	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	19	0.22
(1,519)	1:83:A:PRO:HD2	1:83:A:PRO:HD3	20	0.22
(1,519)	1:83:A:PRO:HD3	1:83:A:PRO:HD2	20	0.22
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	13	0.22
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	13	0.22
(1,417)	1:37:A:VAL:HG23	1:73:A:THR:HG21	4	0.22
(1,417)	1:37:A:VAL:HG22	1:73:A:THR:HG1	16	0.22
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	20	0.22
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	1	0.22
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	1	0.22
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	1	0.22
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	6	0.22
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	6	0.22
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	11	0.22
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	11	0.22
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	11	0.22
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	13	0.22
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	13	0.22
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	13	0.22
(1,312)	1:58:A:ILE:HG23	1:57:A:THR:HB	11	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	5	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	5	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	7	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	7	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	9	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	9	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	19	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	19	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	20	0.22
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	20	0.22
(1,278)	1:48:A:LYS:HD3	1:43:A:ILE:HG21	1	0.22
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	4	0.22
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	5	0.22
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	10	0.22
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	16	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	4	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	4	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	4	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	4	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	9	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	9	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	9	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	9	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	17	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	17	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	17	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	17	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	18	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	18	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	18	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	18	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	20	0.22
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	20	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	20	0.22
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	4	0.22
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	4	0.22
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	1	0.22
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	1	0.22
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	6	0.22
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	6	0.22
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	19	0.22
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	19	0.22
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	13	0.22
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	13	0.22
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	17	0.22
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	17	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	1	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	1	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	4	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	4	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	5	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	5	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	6	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	6	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	7	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	7	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	8	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	8	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	9	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	9	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	10	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	10	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	11	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	11	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	12	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	12	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	13	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	13	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	14	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	14	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	16	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	16	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	18	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	18	0.22
(1,156)	1:26:A:SER:HB2	1:26:A:SER:HB3	19	0.22
(1,156)	1:26:A:SER:HB3	1:26:A:SER:HB2	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	18	0.22
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	18	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	12	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	12	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	13	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	13	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	15	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	15	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	16	0.22
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	16	0.22
(1,66)	1:17:A:THR:HG1	1:16:A:LYS:HB2	6	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	1	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	1	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	2	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	2	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	3	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	3	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	4	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	4	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	5	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	5	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	6	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	6	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	7	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	7	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	8	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	8	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	9	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	9	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	10	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	10	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	11	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	11	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	12	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	12	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	13	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	13	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	14	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	14	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	15	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	15	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	16	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	17	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	17	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	18	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	18	0.22
(1,51)	1:11:A:ASP:HB2	1:11:A:ASP:HB3	20	0.22
(1,51)	1:11:A:ASP:HB3	1:11:A:ASP:HB2	20	0.22
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG21	5	0.22
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	2	0.21
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	10	0.21
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	10	0.21
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	9	0.21
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	9	0.21
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	13	0.21
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	13	0.21
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	3	0.21
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	5	0.21
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	9	0.21
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	19	0.21
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	4	0.21
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	4	0.21
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	13	0.21
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	13	0.21
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	2	0.21
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	5	0.21
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	8	0.21
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	3	0.21
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	17	0.21
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	20	0.21
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	20	0.21
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	11	0.21
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	11	0.21
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	20	0.21
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	20	0.21
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	2	0.21
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	4	0.21
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	7	0.21
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	9	0.21
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	10	0.21
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	2	0.21
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	6	0.21
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	12	0.21
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	18	0.21
(1,2764)	1:103:B:THR:HG23	1:105:B:ILE:HB	18	0.21
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	15	0.21
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	15	0.21
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	15	0.21
(1,2376)	1:58:B:ILE:HG21	1:56:B:PRO:HB2	10	0.21
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	5	0.21
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	5	0.21
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	5	0.21
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	5	0.21
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	5	0.21
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	5	0.21
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	19	0.21
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	19	0.21
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	19	0.21
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	5	0.21
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	5	0.21
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	8	0.21
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	8	0.21
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	19	0.21
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	19	0.21
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	20	0.21
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	20	0.21
(1,1978)	1:89:B:THR:HG23	1:90:B:PHE:HB2	13	0.21
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	17	0.21
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	17	0.21
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	17	0.21
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	17	0.21
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	17	0.21
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	17	0.21
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	17	0.21
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	17	0.21
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	17	0.21
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	17	0.21
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	17	0.21
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	17	0.21
(1,1965)	1:58:B:ILE:HG21	1:90:B:PHE:HD1	10	0.21
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD11	9	0.21
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	6	0.21
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	6	0.21
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	2	0.21
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	13	0.21
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	13	0.21
(1,1804)	1:73:B:THR:HG22	1:39:B:PRO:HG3	15	0.21
(1,1800)	1:37:B:VAL:HG21	1:73:B:THR:HG21	18	0.21
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	6	0.21
(1,1725)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	9	0.21
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	2	0.21
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	2	0.21
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	2	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	1	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	1	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	3	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	3	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	6	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	6	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	7	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	7	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	9	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	9	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	17	0.21
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	17	0.21
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	6	0.21
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	7	0.21
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	12	0.21
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	12	0.21
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE1	17	0.21
(1,1636)	1:41:B:THR:HB	1:20:B:TYR:HE2	17	0.21
(1,1570)	1:34:B:THR:HA	1:34:B:THR:HG22	13	0.21
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	6	0.21
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	6	0.21
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	2	0.21
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	2	0.21
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	13	0.21
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	13	0.21
(1,1403)	1:6:B:LEU:HB3	1:5:B:THR:HG22	2	0.21
(1,1374)	1:103:A:THR:HG22	1:102:A:ILE:HG23	18	0.21
(1,1287)	1:90:A:PHE:HB3	1:94:A:ILE:HG13	18	0.21
(1,983)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	16	0.21
(1,983)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	16	0.21
(1,982)	1:56:A:PRO:HD2	1:56:A:PRO:HD3	16	0.21
(1,982)	1:56:A:PRO:HD3	1:56:A:PRO:HD2	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,790)	1:14:A:SER:HB2	1:14:A:SER:HB3	1	0.21
(1,790)	1:14:A:SER:HB3	1:14:A:SER:HB2	1	0.21
(1,789)	1:14:A:SER:HB2	1:14:A:SER:HB3	1	0.21
(1,789)	1:14:A:SER:HB3	1:14:A:SER:HB2	1	0.21
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	18	0.21
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG13	20	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	2	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	2	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	2	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	2	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	2	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	2	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	12	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	12	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	12	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	12	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	12	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	12	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	13	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	13	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	13	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	13	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	13	0.21
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	13	0.21
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB2	11	0.21
(1,646)	1:94:A:ILE:HA	1:93:A:GLU:HB3	11	0.21
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	2	0.21
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	2	0.21
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	3	0.21
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	3	0.21
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	9	0.21
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	9	0.21
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	11	0.21
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	11	0.21
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	14	0.21
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	14	0.21
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	16	0.21
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	16	0.21
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	8	0.21
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	8	0.21
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	8	0.21
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	8	0.21
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	8	0.21
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	8	0.21
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	8	0.21
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	8	0.21
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	8	0.21
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	8	0.21
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	8	0.21
(1,564)	1:87:A:LEU:HD22	1:60:A:ILE:HG21	17	0.21
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	3	0.21
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	3	0.21
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	3	0.21
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	3	0.21
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	3	0.21
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	3	0.21
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	20	0.21
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	20	0.21
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	20	0.21
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	20	0.21
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	20	0.21
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	20	0.21
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	3	0.21
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	3	0.21
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	19	0.21
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	19	0.21
(1,445)	1:76:A:PRO:HG3	1:34:A:THR:HG23	16	0.21
(1,444)	1:34:A:THR:HG23	1:76:A:PRO:HG3	11	0.21
(1,421)	1:71:A:GLN:HB3	1:73:A:THR:HG23	3	0.21
(1,420)	1:73:A:THR:HG23	1:39:A:PRO:HG3	2	0.21
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	17	0.21
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	20	0.21
(1,340)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	18	0.21
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	18	0.21
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	18	0.21
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	18	0.21
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	5	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	1	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	1	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	2	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	2	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	4	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	6	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	6	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	10	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	10	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	11	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	11	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	12	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	12	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	15	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	15	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	16	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	16	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	17	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	17	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	18	0.21
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	18	0.21
(1,272)	1:46:A:LEU:HB2	1:41:A:THR:HG1	2	0.21
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	8	0.21
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	3	0.21
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	3	0.21
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	3	0.21
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	3	0.21
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	18	0.21
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	2	0.21
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	9	0.21
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	10	0.21
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	11	0.21
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	18	0.21
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	13	0.21
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	13	0.21
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	16	0.21
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	16	0.21
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	14	0.21
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	14	0.21
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	13	0.21
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	13	0.21
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	14	0.21
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	14	0.21
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	7	0.21
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	7	0.21
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	15	0.21
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	7	0.21
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	7	0.21
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	17	0.21
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	17	0.21
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	20	0.21
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	20	0.21
(1,54)	1:10:A:LYS:HD2	1:14:A:SER:HB2	1	0.21
(1,54)	1:10:A:LYS:HD2	1:14:A:SER:HB3	1	0.21
(1,54)	1:10:A:LYS:HD3	1:14:A:SER:HB2	1	0.21
(1,54)	1:10:A:LYS:HD3	1:14:A:SER:HB3	1	0.21
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	17	0.2
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	6	0.2
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	6	0.2
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	7	0.2
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	7	0.2
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	10	0.2
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	10	0.2
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	17	0.2
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	17	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	3	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	3	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	11	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	11	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	12	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	12	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	17	0.2
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	17	0.2
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	12	0.2
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	15	0.2
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	18	0.2
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	20	0.2
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	6	0.2
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	19	0.2
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	18	0.2
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	18	0.2
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	3	0.2
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	3	0.2
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	14	0.2
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	14	0.2
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	7	0.2
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	5	0.2
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	9	0.2
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	9	0.2
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	3	0.2
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	3	0.2
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	3	0.2
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	3	0.2
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	16	0.2
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	16	0.2
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	5	0.2
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	13	0.2
(1,2764)	1:103:B:THR:HG21	1:105:B:ILE:HB	4	0.2
(1,2413)	1:43:B:ILE:HG13	1:64:B:ASP:HB2	15	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	1	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	1	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	1	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	1	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	1	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	1	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	10	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	10	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	10	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	10	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	10	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	10	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	11	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	11	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	11	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	11	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	11	0.2
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	11	0.2
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	1	0.2
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	1	0.2
(1,2053)	1:69:B:THR:HG1	1:98:B:ILE:H	2	0.2
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	12	0.2
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	12	0.2
(1,1978)	1:89:B:THR:HG21	1:90:B:PHE:HB2	18	0.2
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	20	0.2
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	20	0.2
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	20	0.2
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	20	0.2
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	20	0.2
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	20	0.2
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	20	0.2
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	20	0.2
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	20	0.2
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	20	0.2
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	20	0.2
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	15	0.2
(1,1948)	1:87:B:LEU:HD21	1:60:B:ILE:HG21	3	0.2
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	16	0.2
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	16	0.2
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	16	0.2
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	16	0.2
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	16	0.2
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	16	0.2
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD1	1	0.2
(1,1941)	1:87:B:LEU:HD11	1:7:B:TYR:HD2	1	0.2
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD1	1	0.2
(1,1941)	1:87:B:LEU:HD12	1:7:B:TYR:HD2	1	0.2
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD1	1	0.2
(1,1941)	1:87:B:LEU:HD13	1:7:B:TYR:HD2	1	0.2
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD1	1	0.2
(1,1941)	1:87:B:LEU:HD21	1:7:B:TYR:HD2	1	0.2
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD1	1	0.2
(1,1941)	1:87:B:LEU:HD22	1:7:B:TYR:HD2	1	0.2
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD1	1	0.2
(1,1941)	1:87:B:LEU:HD23	1:7:B:TYR:HD2	1	0.2
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	8	0.2
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	11	0.2
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	11	0.2
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	11	0.2
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	11	0.2
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	11	0.2
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	11	0.2
(1,1804)	1:73:B:THR:HG22	1:39:B:PRO:HG3	7	0.2
(1,1794)	1:69:B:THR:HG23	1:56:B:PRO:HD3	10	0.2
(1,1772)	1:65:B:PHE:HB3	1:66:B:ILE:HG13	2	0.2
(1,1716)	1:61:B:ASP:HB3	1:60:B:ILE:HG13	3	0.2
(1,1710)	1:60:B:ILE:HG21	1:58:B:ILE:HG12	2	0.2
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	2	0.2
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	2	0.2
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	13	0.2
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	1	0.2
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	1	0.2
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	1	0.2
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	1	0.2
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	18	0.2
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	18	0.2
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	18	0.2
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	18	0.2
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB2	15	0.2
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB3	15	0.2
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	7	0.2
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	8	0.2
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	8	0.2
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	11	0.2
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	11	0.2
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	13	0.2
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	13	0.2
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	14	0.2
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	14	0.2
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	4	0.2
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	4	0.2
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	16	0.2
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	16	0.2
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	17	0.2
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	17	0.2
(1,733)	1:103:A:THR:HG22	1:102:A:ILE:HB	4	0.2
(1,723)	1:98:A:ILE:HD12	1:102:A:ILE:HG12	11	0.2
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	14	0.2
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	14	0.2
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	14	0.2
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	14	0.2
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	14	0.2
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	14	0.2
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	8	0.2
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	8	0.2
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	10	0.2
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	10	0.2
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	5	0.2
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	5	0.2
(1,594)	1:89:A:THR:HG23	1:90:A:PHE:HB2	17	0.2
(1,594)	1:89:A:THR:HG23	1:90:A:PHE:HB2	20	0.2
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	3	0.2
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	3	0.2
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	3	0.2
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	3	0.2
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	3	0.2
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	3	0.2
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	3	0.2
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	3	0.2
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	3	0.2
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	3	0.2
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	3	0.2
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	4	0.2
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	4	0.2
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	4	0.2
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	4	0.2
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	4	0.2
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	4	0.2
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	4	0.2
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	4	0.2
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	4	0.2
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	4	0.2
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	4	0.2
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	4	0.2
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	17	0.2
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	17	0.2
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	17	0.2
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	17	0.2
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	17	0.2
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	17	0.2
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	17	0.2
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	17	0.2
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	17	0.2
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	17	0.2
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	17	0.2
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	17	0.2
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	4	0.2
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	4	0.2
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	4	0.2
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	4	0.2
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	4	0.2
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	4	0.2
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	13	0.2
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	13	0.2
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	13	0.2
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	13	0.2
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	13	0.2
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	13	0.2
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	13	0.2
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	13	0.2
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	13	0.2
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	13	0.2
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	13	0.2
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	14	0.2
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	14	0.2
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	14	0.2
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	14	0.2
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	14	0.2
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	14	0.2
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	14	0.2
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	14	0.2
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	14	0.2
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	14	0.2
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	14	0.2
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	14	0.2
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD1	16	0.2
(1,557)	1:87:A:LEU:HD11	1:7:A:TYR:HD2	16	0.2
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD1	16	0.2
(1,557)	1:87:A:LEU:HD12	1:7:A:TYR:HD2	16	0.2
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD1	16	0.2
(1,557)	1:87:A:LEU:HD13	1:7:A:TYR:HD2	16	0.2
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD1	16	0.2
(1,557)	1:87:A:LEU:HD21	1:7:A:TYR:HD2	16	0.2
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD1	16	0.2
(1,557)	1:87:A:LEU:HD22	1:7:A:TYR:HD2	16	0.2
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD1	16	0.2
(1,557)	1:87:A:LEU:HD23	1:7:A:TYR:HD2	16	0.2
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	4	0.2
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	4	0.2
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	6	0.2
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	6	0.2
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	7	0.2
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	7	0.2
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	15	0.2
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	5	0.2
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	5	0.2
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	5	0.2
(1,420)	1:73:A:THR:HG21	1:39:A:PRO:HG3	13	0.2
(1,420)	1:73:A:THR:HG21	1:39:A:PRO:HG3	18	0.2
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	16	0.2
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	14	0.2
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	14	0.2
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	14	0.2
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB2	6	0.2
(1,160)	1:28:A:LEU:HA	1:26:A:SER:HB3	6	0.2
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	2	0.2
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	2	0.2
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	12	0.2
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	12	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	4	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	4	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	6	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	6	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	9	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	9	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	10	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	10	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	19	0.2
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	19	0.2
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	12	0.19
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	12	0.19
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	14	0.19
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	14	0.19
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	15	0.19
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	15	0.19
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	6	0.19
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	6	0.19
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	8	0.19
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	18	0.19
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	18	0.19
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	20	0.19
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	20	0.19
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	11	0.19
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	14	0.19
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	14	0.19
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	14	0.19
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	13	0.19
(1,3039)	1:7:B:TYR:H	1:23:B:ASP:H	17	0.19
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	20	0.19
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	14	0.19
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	14	0.19
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	13	0.19
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	13	0.19
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	15	0.19
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	15	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	5	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	5	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	13	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	13	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	14	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	14	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	15	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	15	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	20	0.19
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	20	0.19
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	10	0.19
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	13	0.19
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	16	0.19
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	19	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	2	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	2	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	3	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	3	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	8	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	8	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	14	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	14	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	17	0.19
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	17	0.19
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	1	0.19
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	1	0.19
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	17	0.19
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	17	0.19
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	1	0.19
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	17	0.19
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	7	0.19
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	5	0.19
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	5	0.19
(1,2067)	1:99:B:ASP:HB2	1:98:B:ILE:HB	11	0.19
(1,2067)	1:99:B:ASP:HB3	1:98:B:ILE:HB	11	0.19
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	2	0.19
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	2	0.19
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	2	0.19
(1,2031)	1:93:B:GLU:HG2	1:94:B:ILE:HG12	4	0.19
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	16	0.19
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	16	0.19
(1,1978)	1:89:B:THR:HG23	1:90:B:PHE:HB2	7	0.19
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	14	0.19
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	14	0.19
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	14	0.19
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	14	0.19
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	14	0.19
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	14	0.19
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	14	0.19
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	14	0.19
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	14	0.19
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	14	0.19
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	14	0.19
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	14	0.19
(1,1948)	1:87:B:LEU:HD22	1:60:B:ILE:HG21	20	0.19
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	17	0.19
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	17	0.19
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	17	0.19
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	17	0.19
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	17	0.19
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	17	0.19
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	18	0.19
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	18	0.19
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	18	0.19
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	18	0.19
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	18	0.19
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	18	0.19
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	15	0.19
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	15	0.19
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	5	0.19
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	5	0.19
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	5	0.19
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	5	0.19
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	5	0.19
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	5	0.19
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	5	0.19
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	5	0.19
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	5	0.19
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	5	0.19
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	5	0.19
(1,1892)	1:82:B:GLU:HB2	1:11:B:ASP:HA	5	0.19
(1,1892)	1:82:B:GLU:HB3	1:11:B:ASP:HA	5	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	4	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	4	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	14	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	14	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	17	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	17	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	20	0.19
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	20	0.19
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG23	6	0.19
(1,1804)	1:73:B:THR:HG23	1:39:B:PRO:HG3	5	0.19
(1,1804)	1:73:B:THR:HG21	1:39:B:PRO:HG3	6	0.19
(1,1804)	1:73:B:THR:HG23	1:39:B:PRO:HG3	8	0.19
(1,1765)	1:66:B:ILE:HG21	1:43:B:ILE:HG13	17	0.19
(1,1764)	1:66:B:ILE:HG21	1:43:B:ILE:HD13	12	0.19
(1,1725)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	3	0.19
(1,1725)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	19	0.19
(1,1722)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	10	0.19
(1,1686)	1:57:B:THR:HG1	1:43:B:ILE:HB	6	0.19
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	8	0.19
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	8	0.19
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB2	19	0.19
(1,1667)	1:47:B:ASP:HA	1:48:B:LYS:HB3	19	0.19
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	3	0.19
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	3	0.19
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	3	0.19
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	3	0.19
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG22	12	0.19
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	13	0.19
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	15	0.19
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	16	0.19
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	19	0.19
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB2	4	0.19
(1,1566)	1:33:B:ASN:HA	1:32:B:LEU:HB3	4	0.19
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	14	0.19
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	14	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	1	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	1	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	3	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	3	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	7	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	7	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	8	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	8	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	10	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	10	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	16	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	16	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	18	0.19
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	18	0.19
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	11	0.19
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	11	0.19
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	18	0.19
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	18	0.19
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB2	20	0.19
(1,1462)	1:19:B:PRO:HA	1:14:B:SER:HB3	20	0.19
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	12	0.19
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	12	0.19
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	13	0.19
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	13	0.19
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	5	0.19
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	5	0.19
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	6	0.19
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	6	0.19
(1,1159)	1:79:A:ILE:HG12	1:76:A:PRO:HD2	14	0.19
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	16	0.19
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	16	0.19
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	16	0.19
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	17	0.19
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	6	0.19
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	6	0.19
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	6	0.19
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	6	0.19
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	6	0.19
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	2	0.19
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	2	0.19
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	6	0.19
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	6	0.19
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	11	0.19
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	11	0.19
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	13	0.19
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	13	0.19
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	16	0.19
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	16	0.19
(1,683)	1:99:A:ASP:HB2	1:98:A:ILE:HB	20	0.19
(1,683)	1:99:A:ASP:HB3	1:98:A:ILE:HB	20	0.19
(1,639)	1:94:A:ILE:HG21	1:4:A:PHE:HE1	16	0.19
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	18	0.19
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	18	0.19
(1,594)	1:89:A:THR:HG1	1:90:A:PHE:HB2	18	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	3	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	3	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	9	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	9	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	11	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	11	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	18	0.19
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	18	0.19
(1,473)	1:79:A:ILE:HG13	1:76:A:PRO:HB2	6	0.19
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG21	9	0.19
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	18	0.19
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	11	0.19
(1,388)	1:65:A:PHE:HB3	1:66:A:ILE:HG13	6	0.19
(1,338)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	4	0.19
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	3	0.19
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	3	0.19
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB2	13	0.19
(1,283)	1:47:A:ASP:HA	1:48:A:LYS:HB3	13	0.19
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	8	0.19
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	8	0.19
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	8	0.19
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	8	0.19
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	19	0.19
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	19	0.19
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	19	0.19
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	9	0.19
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	9	0.19
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE1	20	0.19
(1,252)	1:41:A:THR:HB	1:20:A:TYR:HE2	20	0.19
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	14	0.19
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	20	0.19
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	8	0.19
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	8	0.19
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	16	0.19
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	16	0.19
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	19	0.19
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	19	0.19
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB2	4	0.19
(1,115)	1:22:A:VAL:HB	1:21:A:PHE:HB3	4	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	1	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	1	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	9	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	9	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	16	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	16	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	20	0.19
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	20	0.19
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	2	0.19
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	2	0.19
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	11	0.19
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	11	0.19
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	14	0.19
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	14	0.19
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	7	0.19
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	7	0.19
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	16	0.19
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	16	0.19
(1,3179)	1:58:B:ILE:H	1:58:B:ILE:HG21	4	0.18
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	5	0.18
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	5	0.18
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	16	0.18
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	16	0.18
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	16	0.18
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	16	0.18
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	12	0.18
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	16	0.18
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	16	0.18
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	11	0.18
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	12	0.18
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	17	0.18
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	11	0.18
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	11	0.18
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	13	0.18
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	13	0.18
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	20	0.18
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	20	0.18
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	10	0.18
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	10	0.18
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	12	0.18
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	12	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	2	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	2	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	3	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	3	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	6	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	6	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	12	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	12	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	16	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	16	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	18	0.18
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	18	0.18
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	1	0.18
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	11	0.18
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	14	0.18
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	20	0.18
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	5	0.18
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	8	0.18
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	11	0.18
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	16	0.18
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	19	0.18
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	13	0.18
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	13	0.18
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	16	0.18
(1,2781)	1:7:A:TYR:H	1:23:A:ASP:H	19	0.18
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	8	0.18
(1,2543)	1:79:B:ILE:HG12	1:76:B:PRO:HD2	19	0.18
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	19	0.18
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	19	0.18
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	19	0.18
(1,2348)	1:42:B:PRO:HB2	1:45:B:LEU:HG	13	0.18
(1,2348)	1:42:B:PRO:HB3	1:45:B:LEU:HG	13	0.18
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	3	0.18
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	9	0.18
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	18	0.18
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	18	0.18
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	18	0.18
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	18	0.18
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	18	0.18
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	18	0.18
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	6	0.18
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	6	0.18
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	6	0.18
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	18	0.18
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	18	0.18
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	18	0.18
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	14	0.18
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	14	0.18
(1,1978)	1:89:B:THR:HG23	1:90:B:PHE:HB2	8	0.18
(1,1978)	1:89:B:THR:HG1	1:90:B:PHE:HB2	16	0.18
(1,1965)	1:58:B:ILE:HG13	1:90:B:PHE:HD2	12	0.18
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	14	0.18
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	14	0.18
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	14	0.18
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	14	0.18
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	14	0.18
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	14	0.18
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	13	0.18
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	13	0.18
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	13	0.18
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	13	0.18
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	13	0.18
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	13	0.18
(1,1928)	1:85:B:ASN:HB3	1:60:B:ILE:HG23	10	0.18
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	5	0.18
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	5	0.18
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	12	0.18
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	5	0.18
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	5	0.18
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	16	0.18
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	16	0.18
(1,1804)	1:73:B:THR:HG21	1:39:B:PRO:HG3	3	0.18
(1,1721)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	2	0.18
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG21	10	0.18
(1,1662)	1:48:B:LYS:HD3	1:43:B:ILE:HG21	3	0.18
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	7	0.18
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	7	0.18
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	7	0.18
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	7	0.18
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG21	1	0.18
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	8	0.18
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	9	0.18
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	10	0.18
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	2	0.18
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	2	0.18
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	5	0.18
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	5	0.18
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	16	0.18
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	16	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	4	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	4	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	12	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	12	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	19	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	19	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	20	0.18
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	20	0.18
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	6	0.18
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	6	0.18
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	13	0.18
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	13	0.18
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	13	0.18
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	13	0.18
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	13	0.18
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	13	0.18
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	13	0.18
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	13	0.18
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	13	0.18
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	13	0.18
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	13	0.18
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	13	0.18
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	13	0.18
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	13	0.18
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	4	0.18
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	4	0.18
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	4	0.18
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	4	0.18
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	20	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	16	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	16	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	16	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	16	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	16	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	16	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	19	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	19	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	19	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	19	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	19	0.18
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	19	0.18
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	8	0.18
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	8	0.18
(1,568)	1:87:A:LEU:HD11	1:87:A:LEU:HA	4	0.18
(1,568)	1:87:A:LEU:HD12	1:87:A:LEU:HA	4	0.18
(1,568)	1:87:A:LEU:HD13	1:87:A:LEU:HA	4	0.18
(1,568)	1:87:A:LEU:HD21	1:87:A:LEU:HA	4	0.18
(1,568)	1:87:A:LEU:HD22	1:87:A:LEU:HA	4	0.18
(1,568)	1:87:A:LEU:HD23	1:87:A:LEU:HA	4	0.18
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	19	0.18
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	19	0.18
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	13	0.18
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	13	0.18
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD1	1	0.18
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD2	1	0.18
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD1	1	0.18
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD2	1	0.18
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD1	1	0.18
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD2	1	0.18
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD1	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD2	1	0.18
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD1	1	0.18
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD2	1	0.18
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD1	1	0.18
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD2	1	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	8	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	8	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	14	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	14	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	17	0.18
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	17	0.18
(1,444)	1:34:A:THR:HG22	1:76:A:PRO:HG3	3	0.18
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	1	0.18
(1,417)	1:37:A:VAL:HG21	1:73:A:THR:HG21	8	0.18
(1,343)	1:58:A:ILE:HB	1:64:A:ASP:HA	10	0.18
(1,326)	1:60:A:ILE:HG21	1:58:A:ILE:HG12	19	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	3	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	5	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	8	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	12	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	13	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	15	0.18
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	16	0.18
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	18	0.18
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	18	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	3	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	3	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	11	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	11	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	13	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	13	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	14	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	14	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	17	0.18
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	17	0.18
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB2	8	0.18
(1,78)	1:19:A:PRO:HA	1:14:A:SER:HB3	8	0.18
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	20	0.18
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	20	0.18
(1,3094)	1:100:B:PHE:H	1:105:B:ILE:HD11	19	0.17
(1,3094)	1:100:B:PHE:H	1:105:B:ILE:HD12	19	0.17
(1,3094)	1:100:B:PHE:H	1:105:B:ILE:HD13	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	1	0.17
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	1	0.17
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	4	0.17
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	4	0.17
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	18	0.17
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	18	0.17
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	8	0.17
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	8	0.17
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	19	0.17
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	19	0.17
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	1	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	1	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	1	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	4	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	4	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	12	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	12	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	13	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	13	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	17	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	17	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	20	0.17
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	20	0.17
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	4	0.17
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	7	0.17
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	7	0.17
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	7	0.17
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	3	0.17
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	3	0.17
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	11	0.17
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	11	0.17
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	10	0.17
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	13	0.17
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	20	0.17
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	20	0.17
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	12	0.17
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	17	0.17
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	10	0.17
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	2	0.17
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	2	0.17
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	8	0.17
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	8	0.17
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	8	0.17
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	1	0.17
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	1	0.17
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	9	0.17
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	9	0.17
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	19	0.17
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	19	0.17
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	4	0.17
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	9	0.17
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	14	0.17
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	4	0.17
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	4	0.17
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB2	18	0.17
(1,2804)	1:60:A:ILE:H	1:59:A:HIS:HB3	18	0.17
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	17	0.17
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	5	0.17
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	6	0.17
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	13	0.17
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	14	0.17
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	1	0.17
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	4	0.17
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	5	0.17
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	5	0.17
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	5	0.17
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	5	0.17
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	5	0.17
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	5	0.17
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	5	0.17
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	5	0.17
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	5	0.17
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	5	0.17
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	5	0.17
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	5	0.17
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	2	0.17
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	2	0.17
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	2	0.17
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	6	0.17
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	6	0.17
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	6	0.17
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	9	0.17
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	9	0.17
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	13	0.17
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	13	0.17
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	13	0.17
(1,2376)	1:58:B:ILE:HG13	1:56:B:PRO:HB2	3	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	7	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	7	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	7	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	7	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	7	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	7	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	12	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	12	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	12	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	12	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	12	0.17
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	12	0.17
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	3	0.17
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	3	0.17
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	3	0.17
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	12	0.17
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	12	0.17
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	12	0.17
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	11	0.17
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	11	0.17
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	11	0.17
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	11	0.17
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	11	0.17
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	11	0.17
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	11	0.17
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	11	0.17
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	11	0.17
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	11	0.17
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	11	0.17
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	11	0.17
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	18	0.17
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	18	0.17
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	18	0.17
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	18	0.17
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	18	0.17
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	18	0.17
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	18	0.17
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	18	0.17
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	18	0.17
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	18	0.17
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	18	0.17
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	4	0.17
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	4	0.17
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	20	0.17
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	20	0.17
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	10	0.17
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	10	0.17
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	12	0.17
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	12	0.17
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	15	0.17
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	15	0.17
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	7	0.17
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	7	0.17
(1,1804)	1:73:B:THR:HG23	1:39:B:PRO:HG3	1	0.17
(1,1793)	1:69:B:THR:HG1	1:54:B:LEU:HA	7	0.17
(1,1793)	1:69:B:THR:HG1	1:54:B:LEU:HA	13	0.17
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	4	0.17
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	4	0.17
(1,1789)	1:40:B:LEU:HG	1:68:B:LEU:H	15	0.17
(1,1724)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	5	0.17
(1,1722)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	9	0.17
(1,1710)	1:60:B:ILE:HG21	1:58:B:ILE:HG12	1	0.17
(1,1704)	1:58:B:ILE:HB	1:58:B:ILE:H	1	0.17
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	15	0.17
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	1	0.17
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	12	0.17
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	6	0.17
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	6	0.17
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	17	0.17
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	17	0.17
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	5	0.17
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	5	0.17
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	17	0.17
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	17	0.17
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	11	0.17
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	11	0.17
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	5	0.17
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	1	0.17
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	1	0.17
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	1	0.17
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	1	0.17
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	1	0.17
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	1	0.17
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	1	0.17
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	1	0.17
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	1	0.17
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	1	0.17
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	1	0.17
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	1	0.17
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	15	0.17
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	15	0.17
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	15	0.17
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	15	0.17
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	15	0.17
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	15	0.17
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	15	0.17
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	15	0.17
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	15	0.17
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	15	0.17
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	15	0.17
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	15	0.17
(1,992)	1:58:A:ILE:HG13	1:56:A:PRO:HB2	18	0.17
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	5	0.17
(1,737)	1:105:A:ILE:HG13	1:99:A:ASP:HA	9	0.17
(1,701)	1:69:A:THR:HG23	1:101:A:LEU:HB3	6	0.17
(1,701)	1:69:A:THR:HG21	1:101:A:LEU:HB2	19	0.17
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	12	0.17
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	12	0.17
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	12	0.17
(1,604)	1:91:A:ARG:HG2	1:88:A:SER:HA	19	0.17
(1,604)	1:91:A:ARG:HG3	1:88:A:SER:HA	19	0.17
(1,594)	1:89:A:THR:HG1	1:90:A:PHE:HB2	19	0.17
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	9	0.17
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	9	0.17
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	9	0.17
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	9	0.17
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	9	0.17
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	9	0.17
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	9	0.17
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	9	0.17
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	9	0.17
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	9	0.17
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	9	0.17
(1,581)	1:58:A:ILE:HG21	1:90:A:PHE:HD1	1	0.17
(1,581)	1:58:A:ILE:HG23	1:90:A:PHE:HD2	3	0.17
(1,564)	1:87:A:LEU:HD11	1:60:A:ILE:HG21	14	0.17
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD13	6	0.17
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	18	0.17
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	18	0.17
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	18	0.17
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	18	0.17
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	18	0.17
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	18	0.17
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	4	0.17
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	4	0.17
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	5	0.17
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	5	0.17
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	10	0.17
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	10	0.17
(1,444)	1:34:A:THR:HG23	1:76:A:PRO:HG3	18	0.17
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	18	0.17
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	18	0.17
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	18	0.17
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	18	0.17
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	18	0.17
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	18	0.17
(1,420)	1:73:A:THR:HG23	1:39:A:PRO:HG3	10	0.17
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	7	0.17
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	9	0.17
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB2	14	0.17
(1,259)	1:19:A:PRO:HG2	1:42:A:PRO:HB3	14	0.17
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB2	14	0.17
(1,259)	1:19:A:PRO:HG3	1:42:A:PRO:HB3	14	0.17
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	7	0.17
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	17	0.17
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG23	19	0.17
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	11	0.17
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	11	0.17
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB2	20	0.17
(1,182)	1:33:A:ASN:HA	1:32:A:LEU:HB3	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	1	0.17
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	1	0.17
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	2	0.17
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	2	0.17
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	5	0.17
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	5	0.17
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	17	0.17
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	17	0.17
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	2	0.17
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	8	0.17
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	8	0.17
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	16	0.17
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	16	0.17
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	6	0.17
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	6	0.17
(1,3103)	1:9:B:ASN:H	1:8:B:LYS:HA	1	0.16
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	5	0.16
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	7	0.16
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	7	0.16
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	12	0.16
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	12	0.16
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	17	0.16
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	17	0.16
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	4	0.16
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	4	0.16
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	5	0.16
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	5	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	2	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	2	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	3	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	3	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	5	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	5	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	9	0.16
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	9	0.16
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD2	6	0.16
(1,3077)	1:82:B:GLU:H	1:10:B:LYS:HD3	6	0.16
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	2	0.16
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	6	0.16
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	11	0.16
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB2	14	0.16
(1,3062)	1:60:B:ILE:H	1:59:B:HIS:HB3	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	6	0.16
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	16	0.16
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	4	0.16
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	6	0.16
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	1	0.16
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	2	0.16
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	4	0.16
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	16	0.16
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	12	0.16
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	12	0.16
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	4	0.16
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	4	0.16
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	7	0.16
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	7	0.16
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	11	0.16
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	11	0.16
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	8	0.16
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	8	0.16
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	8	0.16
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	19	0.16
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	4	0.16
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	8	0.16
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	11	0.16
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	12	0.16
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	15	0.16
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	17	0.16
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	18	0.16
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	9	0.16
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	6	0.16
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	13	0.16
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	16	0.16
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	1	0.16
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	3	0.16
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	18	0.16
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	19	0.16
(1,2758)	1:103:B:THR:HG1	1:102:B:ILE:HG23	18	0.16
(1,2571)	1:5:B:THR:HG21	1:83:B:PRO:HA	15	0.16
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	5	0.16
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	5	0.16
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	5	0.16
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	7	0.16
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	7	0.16
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	14	0.16
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	14	0.16
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	14	0.16
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	16	0.16
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	16	0.16
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	16	0.16
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	17	0.16
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	17	0.16
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	17	0.16
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	4	0.16
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	4	0.16
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	4	0.16
(1,1988)	1:91:B:ARG:HG2	1:88:B:SER:HA	11	0.16
(1,1988)	1:91:B:ARG:HG3	1:88:B:SER:HA	11	0.16
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	8	0.16
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	8	0.16
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	8	0.16
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	8	0.16
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	8	0.16
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	8	0.16
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	8	0.16
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	8	0.16
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	8	0.16
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	8	0.16
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	8	0.16
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	8	0.16
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD13	2	0.16
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	11	0.16
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	11	0.16
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	6	0.16
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	6	0.16
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	18	0.16
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	18	0.16
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	19	0.16
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	19	0.16
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	10	0.16
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	10	0.16
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	11	0.16
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	11	0.16
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	5	0.16
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	12	0.16
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	12	0.16
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	14	0.16
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	14	0.16
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	14	0.16
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	14	0.16
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	14	0.16
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	14	0.16
(1,1804)	1:73:B:THR:HG21	1:39:B:PRO:HG3	9	0.16
(1,1793)	1:69:B:THR:HG1	1:54:B:LEU:HA	4	0.16
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	13	0.16
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	13	0.16
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	18	0.16
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	18	0.16
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD13	5	0.16
(1,1710)	1:60:B:ILE:HG21	1:58:B:ILE:HG12	9	0.16
(1,1710)	1:60:B:ILE:HG21	1:58:B:ILE:HG12	10	0.16
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	11	0.16
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	11	0.16
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	11	0.16
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	15	0.16
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	15	0.16
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	15	0.16
(1,1662)	1:48:B:LYS:HD3	1:43:B:ILE:HG21	2	0.16
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	7	0.16
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	18	0.16
(1,1645)	1:43:B:ILE:HG13	1:42:B:PRO:HA	1	0.16
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	20	0.16
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	20	0.16
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	20	0.16
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	20	0.16
(1,1635)	1:19:B:PRO:HG2	1:41:B:THR:HB	4	0.16
(1,1635)	1:19:B:PRO:HG3	1:41:B:THR:HB	4	0.16
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	12	0.16
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	12	0.16
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	15	0.16
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	15	0.16
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	3	0.16
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	4	0.16
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	20	0.16
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	4	0.16
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	18	0.16
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	18	0.16
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	15	0.16
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	15	0.16
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	6	0.16
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	6	0.16
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	9	0.16
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	9	0.16
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	15	0.16
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	15	0.16
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	16	0.16
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	16	0.16
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	7	0.16
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	7	0.16
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	17	0.16
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	17	0.16
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	7	0.16
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	7	0.16
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	20	0.16
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	20	0.16
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	17	0.16
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	17	0.16
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	17	0.16
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	17	0.16
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	17	0.16
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	17	0.16
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	17	0.16
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	17	0.16
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	17	0.16
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	17	0.16
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	17	0.16
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	17	0.16
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	17	0.16
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	17	0.16
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	17	0.16
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	17	0.16
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	17	0.16
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	17	0.16
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	17	0.16
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	17	0.16
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	17	0.16
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	17	0.16
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	17	0.16
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	17	0.16
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	17	0.16
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	17	0.16
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	17	0.16
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	17	0.16
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	17	0.16
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	17	0.16
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	17	0.16
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	17	0.16
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	17	0.16
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	17	0.16
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	17	0.16
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	2	0.16
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	2	0.16
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	2	0.16
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	10	0.16
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	10	0.16
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	10	0.16
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	18	0.16
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	18	0.16
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	18	0.16
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	19	0.16
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	19	0.16
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	19	0.16
(1,669)	1:69:A:THR:HG1	1:98:A:ILE:H	3	0.16
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	18	0.16
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	18	0.16
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	18	0.16
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	18	0.16
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	18	0.16
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	18	0.16
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	18	0.16
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	18	0.16
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	18	0.16
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	18	0.16
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	18	0.16
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	18	0.16
(1,581)	1:58:A:ILE:HG21	1:90:A:PHE:HD1	12	0.16
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	5	0.16
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	5	0.16
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	5	0.16
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	5	0.16
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	5	0.16
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	8	0.16
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	8	0.16
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	10	0.16
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	10	0.16
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	13	0.16
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	13	0.16
(1,508)	1:82:A:GLU:HB2	1:11:A:ASP:HA	1	0.16
(1,508)	1:82:A:GLU:HB3	1:11:A:ASP:HA	1	0.16
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	2	0.16
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	2	0.16
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	15	0.16
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	15	0.16
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG11	11	0.16
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG12	11	0.16
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG13	11	0.16
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG21	11	0.16
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG22	11	0.16
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG23	11	0.16
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG11	11	0.16
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG12	11	0.16
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG13	11	0.16
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG21	11	0.16
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG22	11	0.16
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG23	11	0.16
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG11	11	0.16
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG12	11	0.16
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG13	11	0.16
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG21	11	0.16
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG22	11	0.16
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG23	11	0.16
(1,471)	1:79:A:ILE:HD11	1:75:A:VAL:HA	11	0.16
(1,471)	1:79:A:ILE:HD12	1:75:A:VAL:HA	11	0.16
(1,471)	1:79:A:ILE:HD13	1:75:A:VAL:HA	11	0.16
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	4	0.16
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	4	0.16
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	9	0.16
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	9	0.16
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	10	0.16
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	4	0.16
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	7	0.16
(1,420)	1:73:A:THR:HG23	1:39:A:PRO:HG3	12	0.16
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	19	0.16
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	12	0.16
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	13	0.16
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	5	0.16
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	5	0.16
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	5	0.16
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	5	0.16
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	5	0.16
(1,312)	1:58:A:ILE:HG13	1:57:A:THR:HB	20	0.16
(1,311)	1:58:A:ILE:HG13	1:57:A:THR:HB	10	0.16
(1,311)	1:58:A:ILE:HG13	1:57:A:THR:HB	20	0.16
(1,302)	1:57:A:THR:HG1	1:43:A:ILE:HB	8	0.16
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	6	0.16
(1,250)	1:41:A:THR:HB	1:17:A:THR:HG23	14	0.16
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	19	0.16
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	19	0.16
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	19	0.16
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	19	0.16
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	19	0.16
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	19	0.16
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	19	0.16
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	19	0.16
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	19	0.16
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	19	0.16
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	19	0.16
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	19	0.16
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	19	0.16
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	19	0.16
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	4	0.16
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	6	0.16
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG21	5	0.16
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG21	8	0.16
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	3	0.16
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	3	0.16
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	12	0.16
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	12	0.16
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	12	0.16
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	15	0.16
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	15	0.16
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	4	0.16
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	4	0.16
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	19	0.16
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	19	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	2	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	2	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	6	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	6	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	14	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	14	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	19	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	19	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	20	0.16
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	20	0.16
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	2	0.16
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	2	0.16
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	14	0.16
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	14	0.16
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	20	0.16
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	20	0.16
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	12	0.16
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	12	0.16
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	7	0.15
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	18	0.15
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	2	0.15
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	2	0.15
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	11	0.15
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	11	0.15
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	11	0.15
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	11	0.15
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	1	0.15
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	1	0.15
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	13	0.15
(1,3052)	1:36:B:LEU:H	1:26:B:SER:H	5	0.15
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	6	0.15
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	14	0.15
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	10	0.15
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	3	0.15
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	5	0.15
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	16	0.15
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	20	0.15
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	7	0.15
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	17	0.15
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	1	0.15
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	17	0.15
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	17	0.15
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	18	0.15
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	18	0.15
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	10	0.15
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	16	0.15
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	2	0.15
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	20	0.15
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	2	0.15
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	20	0.15
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	19	0.15
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	19	0.15
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	9	0.15
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	10	0.15
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	11	0.15
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	14	0.15
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	20	0.15
(1,2764)	1:103:B:THR:HG1	1:105:B:ILE:HB	3	0.15
(1,2764)	1:103:B:THR:HG1	1:105:B:ILE:HB	9	0.15
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	7	0.15
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	7	0.15
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	7	0.15
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	7	0.15
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	7	0.15
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	7	0.15
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	7	0.15
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	7	0.15
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	7	0.15
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	7	0.15
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	7	0.15
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	7	0.15
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	9	0.15
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	9	0.15
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	9	0.15
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	9	0.15
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	9	0.15
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	9	0.15
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	9	0.15
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	9	0.15
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	9	0.15
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	9	0.15
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	9	0.15
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	13	0.15
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	13	0.15
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	13	0.15
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	13	0.15
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	13	0.15
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	13	0.15
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	13	0.15
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	13	0.15
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	13	0.15
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	13	0.15
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	13	0.15
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	13	0.15
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	1	0.15
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	1	0.15
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	1	0.15
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	4	0.15
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	4	0.15
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	4	0.15
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	8	0.15
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	8	0.15
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	8	0.15
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	11	0.15
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	11	0.15
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	11	0.15
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	12	0.15
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	12	0.15
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	12	0.15
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	18	0.15
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	18	0.15
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	18	0.15
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	18	0.15
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	9	0.15
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	9	0.15
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	9	0.15
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	16	0.15
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	16	0.15
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	3	0.15
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	3	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	3	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	3	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	3	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	3	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	3	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	3	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	3	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	3	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	3	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	3	0.15
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	16	0.15
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	16	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	16	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	16	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	16	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	16	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	16	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	16	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	16	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	16	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	16	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	16	0.15
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	19	0.15
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	19	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	19	0.15
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	19	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	19	0.15
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	19	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	19	0.15
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	19	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	19	0.15
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	19	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	19	0.15
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	19	0.15
(1,1965)	1:58:B:ILE:HG23	1:90:B:PHE:HD2	20	0.15
(1,1961)	1:90:B:PHE:HE1	1:57:B:THR:HB	8	0.15
(1,1961)	1:90:B:PHE:HE2	1:57:B:THR:HB	8	0.15
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	3	0.15
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	3	0.15
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	3	0.15
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	3	0.15
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	3	0.15
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	12	0.15
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	12	0.15
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	12	0.15
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	12	0.15
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	12	0.15
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	12	0.15
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	17	0.15
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	17	0.15
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	17	0.15
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	17	0.15
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	17	0.15
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	17	0.15
(1,1948)	1:87:B:LEU:HD22	1:60:B:ILE:HG21	12	0.15
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	4	0.15
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	4	0.15
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	4	0.15
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	4	0.15
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	4	0.15
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	4	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	1	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	1	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	8	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	8	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	14	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	14	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	17	0.15
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	17	0.15
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	2	0.15
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	2	0.15
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	2	0.15
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	2	0.15
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	2	0.15
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	2	0.15
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	2	0.15
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	2	0.15
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	2	0.15
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	2	0.15
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	2	0.15
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB2	7	0.15
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB3	7	0.15
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	1	0.15
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	1	0.15
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	3	0.15
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	3	0.15
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	6	0.15
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	6	0.15
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	6	0.15
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	14	0.15
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	14	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG11	3	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG12	3	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG13	3	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG21	3	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG22	3	0.15
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG23	3	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG11	3	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG12	3	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG13	3	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG21	3	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG22	3	0.15
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG23	3	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG11	3	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG12	3	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG13	3	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG21	3	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG22	3	0.15
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG23	3	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	2	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	2	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	4	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	4	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	9	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	9	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	11	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	11	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	17	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	17	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	20	0.15
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1828)	1:34:B:THR:HG22	1:76:B:PRO:HG3	12	0.15
(1,1828)	1:34:B:THR:HG22	1:76:B:PRO:HG3	20	0.15
(1,1804)	1:73:B:THR:HG22	1:39:B:PRO:HG3	18	0.15
(1,1801)	1:37:B:VAL:HG22	1:73:B:THR:HG22	1	0.15
(1,1800)	1:37:B:VAL:HG22	1:73:B:THR:HG1	10	0.15
(1,1795)	1:69:B:THR:HG1	1:69:B:THR:HA	2	0.15
(1,1765)	1:66:B:ILE:HG13	1:43:B:ILE:HG21	20	0.15
(1,1747)	1:43:B:ILE:HG13	1:65:B:PHE:HD1	1	0.15
(1,1722)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	19	0.15
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	16	0.15
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	16	0.15
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	16	0.15
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	1	0.15
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	14	0.15
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG13	3	0.15
(1,1663)	1:43:B:ILE:HG21	1:48:B:LYS:HG2	17	0.15
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	17	0.15
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	19	0.15
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	14	0.15
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	9	0.15
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	9	0.15
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB2	1	0.15
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB3	1	0.15
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	1	0.15
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	1	0.15
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	1	0.15
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	1	0.15
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	1	0.15
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	1	0.15
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	1	0.15
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	1	0.15
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	1	0.15
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	1	0.15
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	1	0.15
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	1	0.15
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	6	0.15
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	6	0.15
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	6	0.15
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	6	0.15
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	6	0.15
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	6	0.15
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	6	0.15
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	6	0.15
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	6	0.15
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	6	0.15
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	6	0.15
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	11	0.15
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	11	0.15
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	11	0.15
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	11	0.15
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	11	0.15
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	11	0.15
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	11	0.15
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	11	0.15
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	11	0.15
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	11	0.15
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	11	0.15
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	11	0.15
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	5	0.15
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	11	0.15
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	14	0.15
(1,1570)	1:34:B:THR:HA	1:34:B:THR:HG22	10	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	9	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	9	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	10	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	10	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	13	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	13	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	15	0.15
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	15	0.15
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	2	0.15
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	2	0.15
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	1	0.15
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	1	0.15
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	2	0.15
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	2	0.15
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	14	0.15
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	14	0.15
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	7	0.15
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	7	0.15
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	3	0.15
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	3	0.15
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	8	0.15
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	12	0.15
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	12	0.15
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	19	0.15
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	19	0.15
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	17	0.15
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	17	0.15
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	12	0.15
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	12	0.15
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	12	0.15
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	12	0.15
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	12	0.15
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	12	0.15
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	12	0.15
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	12	0.15
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	12	0.15
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	12	0.15
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	12	0.15
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	12	0.15
(1,1073)	1:56:A:PRO:HD2	1:67:A:MET:HG2	13	0.15
(1,1073)	1:56:A:PRO:HD2	1:67:A:MET:HG3	13	0.15
(1,1073)	1:56:A:PRO:HD3	1:67:A:MET:HG2	13	0.15
(1,1073)	1:56:A:PRO:HD3	1:67:A:MET:HG3	13	0.15
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	1	0.15
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	1	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	1	0.15
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	4	0.15
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	4	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	4	0.15
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	6	0.15
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	6	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	6	0.15
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	11	0.15
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	11	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	11	0.15
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	12	0.15
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	12	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	12	0.15
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	15	0.15
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	15	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	15	0.15
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	20	0.15
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	20	0.15
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	10	0.15
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB3	14	0.15
(1,723)	1:98:A:ILE:HD11	1:102:A:ILE:HG12	10	0.15
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD11	18	0.15
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD12	18	0.15
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD13	18	0.15
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD21	18	0.15
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD22	18	0.15
(1,710)	1:97:A:ALA:HA	1:101:A:LEU:HD23	18	0.15
(1,701)	1:69:A:THR:HG21	1:101:A:LEU:HB3	11	0.15
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	3	0.15
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	3	0.15
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	3	0.15
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	18	0.15
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	18	0.15
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	18	0.15
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	14	0.15
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	14	0.15
(1,585)	1:58:A:ILE:HB	1:90:A:PHE:HZ	20	0.15
(1,575)	1:89:A:THR:HG22	1:87:A:LEU:HB2	11	0.15
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	7	0.15
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	7	0.15
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	7	0.15
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	7	0.15
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	7	0.15
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	7	0.15
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD13	1	0.15
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD12	13	0.15
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	5	0.15
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	5	0.15
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	18	0.15
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	18	0.15
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	15	0.15
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	15	0.15
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	15	0.15
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	15	0.15
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	15	0.15
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	15	0.15
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	15	0.15
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	15	0.15
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	15	0.15
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	15	0.15
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	15	0.15
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	16	0.15
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	16	0.15
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	20	0.15
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	20	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	2	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	2	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	4	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	4	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	5	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	5	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	17	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	17	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	18	0.15
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	18	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG11	6	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG12	6	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG13	6	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG21	6	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG22	6	0.15
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG23	6	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG11	6	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG12	6	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG13	6	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG21	6	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG22	6	0.15
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG23	6	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG11	6	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG12	6	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG13	6	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG21	6	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG22	6	0.15
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG23	6	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	1	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	1	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	8	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	8	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	11	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	12	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	12	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	18	0.15
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	18	0.15
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	9	0.15
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	11	0.15
(1,416)	1:37:A:VAL:HG21	1:73:A:THR:HG21	14	0.15
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	7	0.15
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	14	0.15
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	2	0.15
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	2	0.15
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	3	0.15
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	3	0.15
(1,343)	1:58:A:ILE:HB	1:64:A:ASP:HA	19	0.15
(1,326)	1:60:A:ILE:HG21	1:58:A:ILE:HG12	7	0.15
(1,326)	1:60:A:ILE:HG21	1:58:A:ILE:HG12	11	0.15
(1,306)	1:56:A:PRO:HB2	1:58:A:ILE:HG13	18	0.15
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	3	0.15
(1,248)	1:40:A:LEU:HG	1:40:A:LEU:HB2	4	0.15
(1,248)	1:40:A:LEU:HG	1:40:A:LEU:HB3	4	0.15
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	9	0.15
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	9	0.15
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	9	0.15
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	9	0.15
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	9	0.15
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	9	0.15
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	9	0.15
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	9	0.15
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	9	0.15
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	9	0.15
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	9	0.15
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	9	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	7	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	7	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	9	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	9	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	11	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	11	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	20	0.15
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	20	0.15
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	10	0.15
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:9:A:ASN:HB2	1:15:A:ALA:HA	3	0.15
(1,56)	1:9:A:ASN:HB3	1:15:A:ALA:HA	3	0.15
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	6	0.15
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	6	0.15
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	18	0.15
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	18	0.15
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	6	0.15
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	6	0.15
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	7	0.15
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	7	0.15
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	15	0.15
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	15	0.15
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	1	0.14
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	3	0.14
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	6	0.14
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	16	0.14
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	1	0.14
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	3	0.14
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	3	0.14
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	20	0.14
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	20	0.14
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	6	0.14
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	10	0.14
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	8	0.14
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	8	0.14
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	14	0.14
(1,3052)	1:36:B:LEU:H	1:26:B:SER:H	20	0.14
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	12	0.14
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	12	0.14
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	18	0.14
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	18	0.14
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	11	0.14
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	13	0.14
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	4	0.14
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	8	0.14
(1,3048)	1:34:B:THR:H	1:31:B:ASN:HA	19	0.14
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	6	0.14
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	9	0.14
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	10	0.14
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	11	0.14
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	12	0.14
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	1	0.14
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	7	0.14
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	7	0.14
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	1	0.14
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	1	0.14
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	11	0.14
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	15	0.14
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	16	0.14
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	7	0.14
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	3	0.14
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	6	0.14
(1,2792)	1:36:A:LEU:H	1:24:A:VAL:H	11	0.14
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	17	0.14
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	2	0.14
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	2	0.14
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	14	0.14
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	14	0.14
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	6	0.14
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	12	0.14
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	16	0.14
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	16	0.14
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	16	0.14
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	16	0.14
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	16	0.14
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	16	0.14
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	16	0.14
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	16	0.14
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	16	0.14
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	16	0.14
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	16	0.14
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	16	0.14
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG2	9	0.14
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG3	9	0.14
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG2	9	0.14
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG3	9	0.14
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	3	0.14
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	3	0.14
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	3	0.14
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	10	0.14
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	10	0.14
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	10	0.14
(1,2440)	1:66:B:ILE:HD11	1:66:B:ILE:HA	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2440)	1:66:B:ILE:HD12	1:66:B:ILE:HA	20	0.14
(1,2440)	1:66:B:ILE:HD13	1:66:B:ILE:HA	20	0.14
(1,2206)	1:22:B:VAL:HG11	1:4:B:PHE:HA	10	0.14
(1,2206)	1:22:B:VAL:HG12	1:4:B:PHE:HA	10	0.14
(1,2206)	1:22:B:VAL:HG13	1:4:B:PHE:HA	10	0.14
(1,2206)	1:22:B:VAL:HG21	1:4:B:PHE:HA	10	0.14
(1,2206)	1:22:B:VAL:HG22	1:4:B:PHE:HA	10	0.14
(1,2206)	1:22:B:VAL:HG23	1:4:B:PHE:HA	10	0.14
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	7	0.14
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	7	0.14
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	7	0.14
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	13	0.14
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	13	0.14
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	13	0.14
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	14	0.14
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	14	0.14
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	14	0.14
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	17	0.14
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	17	0.14
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	17	0.14
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	3	0.14
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	3	0.14
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	5	0.14
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	5	0.14
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	5	0.14
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	5	0.14
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	5	0.14
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	5	0.14
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	5	0.14
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	5	0.14
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	5	0.14
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	5	0.14
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	5	0.14
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	5	0.14
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	10	0.14
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	10	0.14
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	10	0.14
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	10	0.14
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	10	0.14
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	10	0.14
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	10	0.14
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	10	0.14
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	10	0.14
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	10	0.14
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	10	0.14
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	4	0.14
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	13	0.14
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	14	0.14
(1,1959)	1:89:B:THR:HG21	1:87:B:LEU:HB2	1	0.14
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	11	0.14
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	11	0.14
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	11	0.14
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	11	0.14
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	11	0.14
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	11	0.14
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	2	0.14
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	2	0.14
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	3	0.14
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	3	0.14
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	9	0.14
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	9	0.14
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD1	13	0.14
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD2	13	0.14
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD1	13	0.14
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD2	13	0.14
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD1	13	0.14
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD2	13	0.14
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD1	13	0.14
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD2	13	0.14
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD1	13	0.14
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD2	13	0.14
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD1	13	0.14
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD2	13	0.14
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	9	0.14
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	9	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	1	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	1	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	2	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	2	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	9	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	9	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	16	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	18	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	18	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	20	0.14
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	20	0.14
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	1	0.14
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	1	0.14
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	10	0.14
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	10	0.14
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	4	0.14
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	4	0.14
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	5	0.14
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	5	0.14
(1,1828)	1:34:B:THR:HG21	1:76:B:PRO:HG3	18	0.14
(1,1795)	1:69:B:THR:HG1	1:69:B:THR:HA	12	0.14
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	2	0.14
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	2	0.14
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	7	0.14
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	7	0.14
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	12	0.14
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	12	0.14
(1,1768)	1:66:B:ILE:HA	1:57:B:THR:HB	1	0.14
(1,1765)	1:66:B:ILE:HG13	1:43:B:ILE:HG21	12	0.14
(1,1722)	1:64:B:ASP:HB3	1:43:B:ILE:HG13	3	0.14
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	1	0.14
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	1	0.14
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	1	0.14
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	15	0.14
(1,1662)	1:48:B:LYS:HD2	1:43:B:ILE:HG21	4	0.14
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG21	1	0.14
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG21	4	0.14
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	5	0.14
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	9	0.14
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	12	0.14
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	12	0.14
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	12	0.14
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	12	0.14
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	19	0.14
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	19	0.14
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB2	2	0.14
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB3	2	0.14
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB2	6	0.14
(1,1622)	1:40:B:LEU:HG	1:20:B:TYR:HB3	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1616)	1:39:B:PRO:HA	1:37:B:VAL:HB	17	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	1	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	1	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	7	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	7	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	8	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	8	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	11	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	11	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	19	0.14
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	19	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	5	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	5	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	6	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	6	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	13	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	13	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	14	0.14
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	14	0.14
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG2	15	0.14
(1,1467)	1:19:B:PRO:HA	1:19:B:PRO:HG3	15	0.14
(1,1450)	1:17:B:THR:HG1	1:16:B:LYS:HB3	10	0.14
(1,1450)	1:17:B:THR:HG1	1:16:B:LYS:HB3	17	0.14
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	8	0.14
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	8	0.14
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	17	0.14
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	17	0.14
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	3	0.14
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	3	0.14
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	10	0.14
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	10	0.14
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	14	0.14
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	14	0.14
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	9	0.14
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	9	0.14
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	16	0.14
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	16	0.14
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	14	0.14
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	14	0.14
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	15	0.14
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	15	0.14
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	6	0.14
(1,1285)	1:94:A:ILE:HG21	1:4:A:PHE:HD1	2	0.14
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	18	0.14
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	18	0.14
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	18	0.14
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	18	0.14
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	18	0.14
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	18	0.14
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	18	0.14
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	18	0.14
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	18	0.14
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	18	0.14
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	18	0.14
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	18	0.14
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	20	0.14
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	20	0.14
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	20	0.14
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	20	0.14
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	20	0.14
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	20	0.14
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	20	0.14
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	20	0.14
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	20	0.14
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	20	0.14
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	20	0.14
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	20	0.14
(1,1157)	1:79:A:ILE:HD11	1:75:A:VAL:HB	6	0.14
(1,1157)	1:79:A:ILE:HD12	1:75:A:VAL:HB	6	0.14
(1,1157)	1:79:A:ILE:HD13	1:75:A:VAL:HB	6	0.14
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	5	0.14
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	5	0.14
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	5	0.14
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	7	0.14
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	7	0.14
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	7	0.14
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	14	0.14
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	14	0.14
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	14	0.14
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	17	0.14
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	17	0.14
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	17	0.14
(1,1048)	1:41:A:THR:HG23	1:66:A:ILE:HB	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,997)	1:58:A:ILE:HA	1:58:A:ILE:HG13	10	0.14
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	8	0.14
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	8	0.14
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	8	0.14
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	8	0.14
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	1	0.14
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	1	0.14
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	1	0.14
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	1	0.14
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	1	0.14
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	1	0.14
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	8	0.14
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	8	0.14
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	8	0.14
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	8	0.14
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	8	0.14
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	8	0.14
(1,733)	1:103:A:THR:HG1	1:102:A:ILE:HB	16	0.14
(1,726)	1:101:A:LEU:HB3	1:102:A:ILE:HG21	10	0.14
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	17	0.14
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	17	0.14
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	17	0.14
(1,641)	1:94:A:ILE:HG13	1:22:A:VAL:HB	12	0.14
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	2	0.14
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	2	0.14
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	3	0.14
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	3	0.14
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	19	0.14
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	19	0.14
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	19	0.14
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	19	0.14
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	19	0.14
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	19	0.14
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	19	0.14
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	19	0.14
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	19	0.14
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	19	0.14
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	19	0.14
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	19	0.14
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	5	0.14
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	5	0.14
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	5	0.14
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	5	0.14
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	5	0.14
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	9	0.14
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	9	0.14
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	9	0.14
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	9	0.14
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	9	0.14
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	9	0.14
(1,564)	1:87:A:LEU:HD11	1:60:A:ILE:HG21	2	0.14
(1,559)	1:87:A:LEU:HD11	1:58:A:ILE:HB	9	0.14
(1,559)	1:87:A:LEU:HD12	1:58:A:ILE:HB	9	0.14
(1,559)	1:87:A:LEU:HD13	1:58:A:ILE:HB	9	0.14
(1,559)	1:87:A:LEU:HD21	1:58:A:ILE:HB	9	0.14
(1,559)	1:87:A:LEU:HD22	1:58:A:ILE:HB	9	0.14
(1,559)	1:87:A:LEU:HD23	1:58:A:ILE:HB	9	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	7	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	7	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	14	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	14	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	15	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	15	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	17	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	17	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	20	0.14
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	20	0.14
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	5	0.14
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	5	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	3	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	3	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	7	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	7	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	10	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	10	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	12	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	12	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	19	0.14
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	19	0.14
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG11	7	0.14
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG12	7	0.14
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG13	7	0.14
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG21	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG22	7	0.14
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG23	7	0.14
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG11	7	0.14
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG12	7	0.14
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG13	7	0.14
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG21	7	0.14
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG22	7	0.14
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG23	7	0.14
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG11	7	0.14
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG12	7	0.14
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG13	7	0.14
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG21	7	0.14
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG22	7	0.14
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG23	7	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	2	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	2	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	5	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	5	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	7	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	7	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	17	0.14
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	17	0.14
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	1	0.14
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	1	0.14
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	1	0.14
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	16	0.14
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	16	0.14
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	20	0.14
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	20	0.14
(1,379)	1:42:A:PRO:HA	1:66:A:ILE:HG13	6	0.14
(1,340)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	16	0.14
(1,327)	1:60:A:ILE:HG12	1:58:A:ILE:HD13	12	0.14
(1,326)	1:60:A:ILE:HG12	1:58:A:ILE:HG12	1	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	1	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	10	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG21	13	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	15	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	16	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG21	17	0.14
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG21	19	0.14
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	6	0.14
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,237)	1:40:A:LEU:HD11	1:20:A:TYR:HE1	15	0.14
(1,237)	1:40:A:LEU:HD11	1:20:A:TYR:HE2	15	0.14
(1,237)	1:40:A:LEU:HD12	1:20:A:TYR:HE1	15	0.14
(1,237)	1:40:A:LEU:HD12	1:20:A:TYR:HE2	15	0.14
(1,237)	1:40:A:LEU:HD13	1:20:A:TYR:HE1	15	0.14
(1,237)	1:40:A:LEU:HD13	1:20:A:TYR:HE2	15	0.14
(1,237)	1:40:A:LEU:HD21	1:20:A:TYR:HE1	15	0.14
(1,237)	1:40:A:LEU:HD21	1:20:A:TYR:HE2	15	0.14
(1,237)	1:40:A:LEU:HD22	1:20:A:TYR:HE1	15	0.14
(1,237)	1:40:A:LEU:HD22	1:20:A:TYR:HE2	15	0.14
(1,237)	1:40:A:LEU:HD23	1:20:A:TYR:HE1	15	0.14
(1,237)	1:40:A:LEU:HD23	1:20:A:TYR:HE2	15	0.14
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	6	0.14
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	6	0.14
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	6	0.14
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	6	0.14
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	6	0.14
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	6	0.14
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	6	0.14
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	6	0.14
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	6	0.14
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	6	0.14
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	6	0.14
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	6	0.14
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	1	0.14
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	10	0.14
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	10	0.14
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	15	0.14
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	15	0.14
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	4	0.14
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	5	0.14
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG11	1	0.14
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG12	1	0.14
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG13	1	0.14
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG21	1	0.14
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG22	1	0.14
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG23	1	0.14
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	2	0.14
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	2	0.14
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	7	0.14
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	7	0.14
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:19:A:PRO:HA	1:19:A:PRO:HG3	8	0.14
(1,66)	1:17:A:THR:HG1	1:16:A:LYS:HB3	19	0.14
(1,56)	1:9:A:ASN:HB2	1:15:A:ALA:HA	12	0.14
(1,56)	1:9:A:ASN:HB3	1:15:A:ALA:HA	12	0.14
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	1	0.14
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	1	0.14
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	10	0.14
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	10	0.14
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	17	0.14
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	17	0.14
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	17	0.14
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	17	0.14
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG2	11	0.13
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG3	11	0.13
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	8	0.13
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	9	0.13
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	11	0.13
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	17	0.13
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	19	0.13
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	3	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	2	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	2	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	6	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	6	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	8	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	8	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	9	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	9	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	14	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	14	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	15	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	15	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	16	0.13
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	16	0.13
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	1	0.13
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	1	0.13
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	2	0.13
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	4	0.13
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	18	0.13
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD1	19	0.13
(1,3084)	1:59:B:HIS:H	1:90:B:PHE:HD2	19	0.13
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	9	0.13
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	10	0.13
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	16	0.13
(1,3067)	1:66:B:ILE:H	1:40:B:LEU:HA	20	0.13
(1,3052)	1:36:B:LEU:H	1:26:B:SER:H	4	0.13
(1,3052)	1:36:B:LEU:H	1:26:B:SER:H	6	0.13
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	15	0.13
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	15	0.13
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	17	0.13
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	17	0.13
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	13	0.13
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	19	0.13
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	15	0.13
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	3	0.13
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	4	0.13
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	5	0.13
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	6	0.13
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	13	0.13
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	19	0.13
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	5	0.13
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	14	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	3	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	3	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	5	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	5	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	9	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	9	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	11	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	11	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	15	0.13
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	15	0.13
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	6	0.13
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	6	0.13
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	19	0.13
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	19	0.13
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	5	0.13
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD1	7	0.13
(1,2826)	1:59:A:HIS:H	1:90:A:PHE:HD2	7	0.13
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	3	0.13
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	11	0.13
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	14	0.13
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	14	0.13
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	13	0.13
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	15	0.13
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	17	0.13
(1,2767)	1:105:B:ILE:HD11	1:105:B:ILE:HA	10	0.13
(1,2767)	1:105:B:ILE:HD12	1:105:B:ILE:HA	10	0.13
(1,2767)	1:105:B:ILE:HD13	1:105:B:ILE:HA	10	0.13
(1,2764)	1:103:B:THR:HG1	1:105:B:ILE:HB	1	0.13
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	6	0.13
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	6	0.13
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	6	0.13
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	6	0.13
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	6	0.13
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	6	0.13
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	6	0.13
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	6	0.13
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	6	0.13
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	6	0.13
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	6	0.13
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	6	0.13
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	9	0.13
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	9	0.13
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	9	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG2	8	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG3	8	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG2	8	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG3	8	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG2	12	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG3	12	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG2	12	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG3	12	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG2	15	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG3	15	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG2	15	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG3	15	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG2	18	0.13
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG3	18	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG2	18	0.13
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG3	18	0.13
(1,2432)	1:41:B:THR:HG23	1:66:B:ILE:HB	18	0.13
(1,2376)	1:58:B:ILE:HG13	1:56:B:PRO:HB2	16	0.13
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	1	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	1	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	1	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	1	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	1	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	1	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	5	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	5	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	5	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	5	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	5	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	5	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	9	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	9	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	9	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	9	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	9	0.13
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	9	0.13
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD11	4	0.13
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD12	4	0.13
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD13	4	0.13
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD21	4	0.13
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD22	4	0.13
(1,2094)	1:97:B:ALA:HA	1:101:B:LEU:HD23	4	0.13
(1,2085)	1:69:B:THR:HG23	1:101:B:LEU:HB3	5	0.13
(1,2053)	1:69:B:THR:HG1	1:98:B:ILE:H	8	0.13
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	8	0.13
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	17	0.13
(1,2010)	1:91:B:ARG:HG2	1:92:B:ASN:HA	15	0.13
(1,2010)	1:91:B:ARG:HG3	1:92:B:ASN:HA	15	0.13
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	5	0.13
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	5	0.13
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	11	0.13
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	11	0.13
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	12	0.13
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	12	0.13
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	17	0.13
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	17	0.13
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	19	0.13
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	19	0.13
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	20	0.13
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	2	0.13
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	2	0.13
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	2	0.13
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	2	0.13
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	2	0.13
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	2	0.13
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	2	0.13
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	2	0.13
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	2	0.13
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	2	0.13
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	2	0.13
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	2	0.13
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	6	0.13
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	6	0.13
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	6	0.13
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	6	0.13
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	6	0.13
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	6	0.13
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	6	0.13
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	6	0.13
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	6	0.13
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	6	0.13
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	6	0.13
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	6	0.13
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	12	0.13
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	12	0.13
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	12	0.13
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	12	0.13
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	12	0.13
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	12	0.13
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	12	0.13
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	12	0.13
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	12	0.13
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	12	0.13
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	12	0.13
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	12	0.13
(1,1965)	1:58:B:ILE:HG21	1:90:B:PHE:HD1	2	0.13
(1,1965)	1:58:B:ILE:HG13	1:90:B:PHE:HD2	3	0.13
(1,1961)	1:90:B:PHE:HE1	1:57:B:THR:HB	19	0.13
(1,1961)	1:90:B:PHE:HE2	1:57:B:THR:HB	19	0.13
(1,1959)	1:89:B:THR:HG21	1:87:B:LEU:HB2	10	0.13
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	6	0.13
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	6	0.13
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	6	0.13
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	6	0.13
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	6	0.13
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	10	0.13
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	10	0.13
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	10	0.13
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	10	0.13
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	10	0.13
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	10	0.13
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	18	0.13
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	18	0.13
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	18	0.13
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	18	0.13
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	18	0.13
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	18	0.13
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	20	0.13
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	20	0.13
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	20	0.13
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	20	0.13
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	20	0.13
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	20	0.13
(1,1943)	1:87:B:LEU:HD11	1:58:B:ILE:HB	3	0.13
(1,1943)	1:87:B:LEU:HD12	1:58:B:ILE:HB	3	0.13
(1,1943)	1:87:B:LEU:HD13	1:58:B:ILE:HB	3	0.13
(1,1943)	1:87:B:LEU:HD21	1:58:B:ILE:HB	3	0.13
(1,1943)	1:87:B:LEU:HD22	1:58:B:ILE:HB	3	0.13
(1,1943)	1:87:B:LEU:HD23	1:58:B:ILE:HB	3	0.13
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	13	0.13
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	13	0.13
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	16	0.13
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	16	0.13
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	12	0.13
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	12	0.13
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	12	0.13
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	12	0.13
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	12	0.13
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	12	0.13
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	12	0.13
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	12	0.13
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	12	0.13
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	12	0.13
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	12	0.13
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB2	11	0.13
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB3	11	0.13
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB2	8	0.13
(1,1867)	1:80:B:LEU:HA	1:7:B:TYR:HB3	8	0.13
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	13	0.13
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	13	0.13
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	17	0.13
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	17	0.13
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	19	0.13
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	19	0.13
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	13	0.13
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	13	0.13
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	14	0.13
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	14	0.13
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	2	0.13
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	2	0.13
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	3	0.13
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	3	0.13
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	8	0.13
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	8	0.13
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	12	0.13
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	12	0.13
(1,1805)	1:71:B:GLN:HB3	1:73:B:THR:HG21	14	0.13
(1,1804)	1:73:B:THR:HG21	1:39:B:PRO:HG3	2	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	1	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	1	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	11	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	11	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	14	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	14	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	16	0.13
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	16	0.13
(1,1765)	1:66:B:ILE:HG13	1:43:B:ILE:HG21	11	0.13
(1,1765)	1:66:B:ILE:HG13	1:43:B:ILE:HG21	16	0.13
(1,1763)	1:42:B:PRO:HA	1:66:B:ILE:HG13	17	0.13
(1,1763)	1:42:B:PRO:HA	1:66:B:ILE:HG13	19	0.13
(1,1727)	1:58:B:ILE:HB	1:64:B:ASP:HA	1	0.13
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	16	0.13
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG21	13	0.13
(1,1635)	1:19:B:PRO:HG2	1:41:B:THR:HB	17	0.13
(1,1635)	1:19:B:PRO:HG3	1:41:B:THR:HB	17	0.13
(1,1635)	1:19:B:PRO:HG2	1:41:B:THR:HB	20	0.13
(1,1635)	1:19:B:PRO:HG3	1:41:B:THR:HB	20	0.13
(1,1623)	1:39:B:PRO:HB2	1:40:B:LEU:HA	7	0.13
(1,1623)	1:39:B:PRO:HB3	1:40:B:LEU:HA	7	0.13
(1,1623)	1:39:B:PRO:HB2	1:40:B:LEU:HA	14	0.13
(1,1623)	1:39:B:PRO:HB3	1:40:B:LEU:HA	14	0.13
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	3	0.13
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	3	0.13
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	3	0.13
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	3	0.13
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	3	0.13
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	3	0.13
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	3	0.13
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	3	0.13
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	3	0.13
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	3	0.13
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	3	0.13
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	3	0.13
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	18	0.13
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	18	0.13
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	18	0.13
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	18	0.13
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	18	0.13
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	18	0.13
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	18	0.13
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	18	0.13
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	18	0.13
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	18	0.13
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	18	0.13
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	18	0.13
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	20	0.13
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	20	0.13
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	20	0.13
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	20	0.13
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	20	0.13
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	20	0.13
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	20	0.13
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	20	0.13
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	20	0.13
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	20	0.13
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	20	0.13
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	3	0.13
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	3	0.13
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	12	0.13
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	12	0.13
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	20	0.13
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	20	0.13
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	10	0.13
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	11	0.13
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	14	0.13
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	7	0.13
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	7	0.13
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	7	0.13
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	7	0.13
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	7	0.13
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	7	0.13
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	5	0.13
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	5	0.13
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	9	0.13
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	9	0.13
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	20	0.13
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	20	0.13
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	4	0.13
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	4	0.13
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	11	0.13
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	11	0.13
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	12	0.13
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	12	0.13
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	13	0.13
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	13	0.13
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	16	0.13
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	16	0.13
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	18	0.13
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	18	0.13
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	19	0.13
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	19	0.13
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	4	0.13
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD11	14	0.13
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD12	14	0.13
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD13	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD11	14	0.13
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD12	14	0.13
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD13	14	0.13
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD11	14	0.13
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD12	14	0.13
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD13	14	0.13
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD11	14	0.13
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD12	14	0.13
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD13	14	0.13
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD11	14	0.13
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD12	14	0.13
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD13	14	0.13
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD11	14	0.13
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD12	14	0.13
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD13	14	0.13
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	6	0.13
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	6	0.13
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	6	0.13
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	6	0.13
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	6	0.13
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	6	0.13
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	6	0.13
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	6	0.13
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	6	0.13
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	6	0.13
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	6	0.13
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	6	0.13
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	3	0.13
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	3	0.13
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	3	0.13
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	3	0.13
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	3	0.13
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	3	0.13
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	3	0.13
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	3	0.13
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	3	0.13
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	3	0.13
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	3	0.13
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	3	0.13
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	3	0.13
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	3	0.13
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	3	0.13
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	3	0.13
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	3	0.13
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	3	0.13
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	3	0.13
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	3	0.13
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	3	0.13
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	3	0.13
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	3	0.13
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	3	0.13
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	3	0.13
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	3	0.13
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	3	0.13
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	3	0.13
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	3	0.13
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	3	0.13
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	3	0.13
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	3	0.13
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	3	0.13
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	3	0.13
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	3	0.13
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	3	0.13
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	3	0.13
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	3	0.13
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	8	0.13
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	8	0.13
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	8	0.13
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	14	0.13
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	14	0.13
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	14	0.13
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	14	0.13
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	17	0.13
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	17	0.13
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	17	0.13
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	17	0.13
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	19	0.13
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	19	0.13
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	19	0.13
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	19	0.13
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	19	0.13
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	19	0.13
(1,822)	1:22:A:VAL:HG11	1:4:A:PHE:HA	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:22:A:VAL:HG12	1:4:A:PHE:HA	3	0.13
(1,822)	1:22:A:VAL:HG13	1:4:A:PHE:HA	3	0.13
(1,822)	1:22:A:VAL:HG21	1:4:A:PHE:HA	3	0.13
(1,822)	1:22:A:VAL:HG22	1:4:A:PHE:HA	3	0.13
(1,822)	1:22:A:VAL:HG23	1:4:A:PHE:HA	3	0.13
(1,730)	1:103:A:THR:HG1	1:99:A:ASP:HB3	1	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD11	7	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD12	7	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD13	7	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD21	7	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD22	7	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD23	7	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD11	8	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD12	8	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD13	8	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD21	8	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD22	8	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD23	8	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD11	9	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD12	9	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD13	9	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD21	9	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD22	9	0.13
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD23	9	0.13
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	5	0.13
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	5	0.13
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	5	0.13
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	20	0.13
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	20	0.13
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	20	0.13
(1,650)	1:91:A:ARG:HB2	1:95:A:ILE:HG13	1	0.13
(1,639)	1:94:A:ILE:HG21	1:4:A:PHE:HE1	11	0.13
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	9	0.13
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	9	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	1	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	1	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	1	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	1	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	1	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	1	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	1	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	1	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	1	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	1	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	1	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	7	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	7	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	7	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	7	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	7	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	7	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	7	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	7	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	7	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	7	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	7	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	7	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	12	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	12	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	12	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	12	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	12	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	12	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	12	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	12	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	12	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	12	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	12	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	12	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	13	0.13
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	13	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	13	0.13
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	13	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	13	0.13
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	13	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	13	0.13
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	13	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	13	0.13
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	13	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	13	0.13
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	13	0.13
(1,585)	1:58:A:ILE:HB	1:90:A:PHE:HZ	4	0.13
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	3	0.13
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	3	0.13
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	3	0.13
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	3	0.13
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	3	0.13
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	12	0.13
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	12	0.13
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	12	0.13
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	12	0.13
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	12	0.13
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	12	0.13
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	17	0.13
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	17	0.13
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	17	0.13
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	17	0.13
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	17	0.13
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	17	0.13
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD23	16	0.13
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	6	0.13
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	6	0.13
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	9	0.13
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	9	0.13
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	5	0.13
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	5	0.13
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	5	0.13
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	5	0.13
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	5	0.13
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	5	0.13
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	5	0.13
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	5	0.13
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	5	0.13
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	5	0.13
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	5	0.13
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	5	0.13
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	12	0.13
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	12	0.13
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	6	0.13
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	6	0.13
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	6	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	1	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	1	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	6	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	8	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	8	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	9	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	9	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	13	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	13	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	20	0.13
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	20	0.13
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD1	20	0.13
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD2	20	0.13
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD1	20	0.13
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD2	20	0.13
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD1	20	0.13
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD2	20	0.13
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	3	0.13
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	3	0.13
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	15	0.13
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	15	0.13
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	19	0.13
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	19	0.13
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	8	0.13
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	8	0.13
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	10	0.13
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	10	0.13
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	12	0.13
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	12	0.13
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	13	0.13
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	13	0.13
(1,420)	1:73:A:THR:HG23	1:39:A:PRO:HG3	3	0.13
(1,420)	1:73:A:THR:HG21	1:39:A:PRO:HG3	6	0.13
(1,420)	1:73:A:THR:HG1	1:39:A:PRO:HG3	16	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	7	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	7	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	9	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	9	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	15	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	15	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	18	0.13
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	18	0.13
(1,343)	1:58:A:ILE:HB	1:64:A:ASP:HA	6	0.13
(1,343)	1:58:A:ILE:HB	1:64:A:ASP:HA	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:64:A:ASP:HB2	1:43:A:ILE:HG13	10	0.13
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	6	0.13
(1,278)	1:48:A:LYS:HD3	1:43:A:ILE:HG21	2	0.13
(1,278)	1:48:A:LYS:HD3	1:43:A:ILE:HG21	12	0.13
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG21	20	0.13
(1,251)	1:19:A:PRO:HG2	1:41:A:THR:HB	20	0.13
(1,251)	1:19:A:PRO:HG3	1:41:A:THR:HB	20	0.13
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	14	0.13
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	14	0.13
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	17	0.13
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	17	0.13
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB2	8	0.13
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB3	8	0.13
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB2	19	0.13
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB3	19	0.13
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	4	0.13
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	4	0.13
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	4	0.13
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	4	0.13
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	4	0.13
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	4	0.13
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	4	0.13
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	4	0.13
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	4	0.13
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	4	0.13
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	4	0.13
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	4	0.13
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	10	0.13
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	10	0.13
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	10	0.13
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	10	0.13
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	10	0.13
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	10	0.13
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	10	0.13
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	10	0.13
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	10	0.13
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	10	0.13
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	10	0.13
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	10	0.13
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	13	0.13
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	13	0.13
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	13	0.13
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	13	0.13
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	13	0.13
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	13	0.13
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	13	0.13
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	13	0.13
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	13	0.13
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	13	0.13
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	13	0.13
(1,232)	1:39:A:PRO:HA	1:37:A:VAL:HB	19	0.13
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	17	0.13
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	17	0.13
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	17	0.13
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	17	0.13
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG21	7	0.13
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	4	0.13
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	4	0.13
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	20	0.13
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	4	0.13
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	4	0.13
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	10	0.13
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	10	0.13
(1,56)	1:9:A:ASN:HB2	1:15:A:ALA:HA	4	0.13
(1,56)	1:9:A:ASN:HB3	1:15:A:ALA:HA	4	0.13
(1,56)	1:9:A:ASN:HB2	1:15:A:ALA:HA	8	0.13
(1,56)	1:9:A:ASN:HB3	1:15:A:ALA:HA	8	0.13
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	13	0.13
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	13	0.13
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	4	0.13
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	4	0.13
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	16	0.13
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	16	0.13
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	19	0.13
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	19	0.13
(1,19)	1:6:A:LEU:HB3	1:5:A:THR:HG21	1	0.13
(1,3141)	1:26:B:SER:H	1:25:B:GLN:HA	18	0.12
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG2	3	0.12
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG3	3	0.12
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	20	0.12
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	9	0.12
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	13	0.12
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	3	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	4	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	5	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	7	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	11	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	14	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	15	0.12
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	18	0.12
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB2	4	0.12
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB3	4	0.12
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB2	18	0.12
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB3	18	0.12
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	4	0.12
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	7	0.12
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	13	0.12
(1,3052)	1:36:B:LEU:H	1:26:B:SER:H	16	0.12
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	10	0.12
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	10	0.12
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	8	0.12
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	12	0.12
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	19	0.12
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB2	2	0.12
(1,3046)	1:32:B:LEU:H	1:2:B:SER:HB3	2	0.12
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	7	0.12
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	8	0.12
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	15	0.12
(1,3038)	1:18:B:TYR:H	1:14:B:SER:HA	18	0.12
(1,2971)	1:81:A:SER:H	1:80:A:LEU:HA	5	0.12
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	2	0.12
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	4	0.12
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	9	0.12
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	18	0.12
(1,2876)	1:20:A:TYR:H	1:19:A:PRO:HG2	14	0.12
(1,2876)	1:20:A:TYR:H	1:19:A:PRO:HG3	14	0.12
(1,2876)	1:20:A:TYR:H	1:19:A:PRO:HG2	18	0.12
(1,2876)	1:20:A:TYR:H	1:19:A:PRO:HG3	18	0.12
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	2	0.12
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	2	0.12
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	9	0.12
(1,2834)	1:103:A:THR:H	1:100:A:PHE:H	13	0.12
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	1	0.12
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	17	0.12
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	10	0.12
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	13	0.12
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	15	0.12
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	18	0.12
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	20	0.12
(1,2814)	1:71:A:GLN:H	1:72:A:MET:HB2	19	0.12
(1,2814)	1:71:A:GLN:H	1:72:A:MET:HB3	19	0.12
(1,2813)	1:67:A:MET:H	1:67:A:MET:HG2	17	0.12
(1,2813)	1:67:A:MET:H	1:67:A:MET:HG3	17	0.12
(1,2810)	1:41:A:THR:H	1:66:A:ILE:HG13	17	0.12
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	4	0.12
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	5	0.12
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	11	0.12
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	9	0.12
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	15	0.12
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	18	0.12
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB2	4	0.12
(1,2793)	1:26:A:SER:H	1:36:A:LEU:HB3	4	0.12
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	1	0.12
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	3	0.12
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	17	0.12
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	18	0.12
(1,2790)	1:34:A:THR:H	1:31:A:ASN:HA	20	0.12
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	8	0.12
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	8	0.12
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	2	0.12
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	7	0.12
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	16	0.12
(1,2780)	1:18:A:TYR:H	1:14:A:SER:HA	18	0.12
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	2	0.12
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	2	0.12
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	2	0.12
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	2	0.12
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	2	0.12
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	2	0.12
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	2	0.12
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	2	0.12
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	2	0.12
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	2	0.12
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	2	0.12
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	14	0.12
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	14	0.12
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	14	0.12
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	14	0.12
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	14	0.12
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	14	0.12
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	14	0.12
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	14	0.12
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	14	0.12
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	14	0.12
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	14	0.12
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	14	0.12
(1,2596)	1:84:B:VAL:HG11	1:8:B:LYS:HB2	6	0.12
(1,2596)	1:84:B:VAL:HG11	1:8:B:LYS:HB3	6	0.12
(1,2596)	1:84:B:VAL:HG12	1:8:B:LYS:HB2	6	0.12
(1,2596)	1:84:B:VAL:HG12	1:8:B:LYS:HB3	6	0.12
(1,2596)	1:84:B:VAL:HG13	1:8:B:LYS:HB2	6	0.12
(1,2596)	1:84:B:VAL:HG13	1:8:B:LYS:HB3	6	0.12
(1,2596)	1:84:B:VAL:HG21	1:8:B:LYS:HB2	6	0.12
(1,2596)	1:84:B:VAL:HG21	1:8:B:LYS:HB3	6	0.12
(1,2596)	1:84:B:VAL:HG22	1:8:B:LYS:HB2	6	0.12
(1,2596)	1:84:B:VAL:HG22	1:8:B:LYS:HB3	6	0.12
(1,2596)	1:84:B:VAL:HG23	1:8:B:LYS:HB2	6	0.12
(1,2596)	1:84:B:VAL:HG23	1:8:B:LYS:HB3	6	0.12
(1,2596)	1:84:B:VAL:HG11	1:8:B:LYS:HB2	15	0.12
(1,2596)	1:84:B:VAL:HG11	1:8:B:LYS:HB3	15	0.12
(1,2596)	1:84:B:VAL:HG12	1:8:B:LYS:HB2	15	0.12
(1,2596)	1:84:B:VAL:HG12	1:8:B:LYS:HB3	15	0.12
(1,2596)	1:84:B:VAL:HG13	1:8:B:LYS:HB2	15	0.12
(1,2596)	1:84:B:VAL:HG13	1:8:B:LYS:HB3	15	0.12
(1,2596)	1:84:B:VAL:HG21	1:8:B:LYS:HB2	15	0.12
(1,2596)	1:84:B:VAL:HG21	1:8:B:LYS:HB3	15	0.12
(1,2596)	1:84:B:VAL:HG22	1:8:B:LYS:HB2	15	0.12
(1,2596)	1:84:B:VAL:HG22	1:8:B:LYS:HB3	15	0.12
(1,2596)	1:84:B:VAL:HG23	1:8:B:LYS:HB2	15	0.12
(1,2596)	1:84:B:VAL:HG23	1:8:B:LYS:HB3	15	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG11	6	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG12	6	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG13	6	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG21	6	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG22	6	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG23	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG11	6	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG12	6	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG13	6	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG21	6	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG22	6	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG23	6	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG11	15	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG12	15	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG13	15	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG21	15	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG22	15	0.12
(1,2595)	1:8:B:LYS:HB2	1:84:B:VAL:HG23	15	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG11	15	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG12	15	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG13	15	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG21	15	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG22	15	0.12
(1,2595)	1:8:B:LYS:HB3	1:84:B:VAL:HG23	15	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG11	6	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG12	6	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG13	6	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG21	6	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG22	6	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG23	6	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG11	6	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG12	6	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG13	6	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG21	6	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG22	6	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG23	6	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG11	15	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG12	15	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG13	15	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG21	15	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG22	15	0.12
(1,2594)	1:8:B:LYS:HB2	1:84:B:VAL:HG23	15	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG11	15	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG12	15	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG13	15	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG21	15	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG22	15	0.12
(1,2594)	1:8:B:LYS:HB3	1:84:B:VAL:HG23	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	2	0.12
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	2	0.12
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	2	0.12
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	12	0.12
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	12	0.12
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	12	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	3	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	3	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	3	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	3	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	3	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	3	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	3	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	3	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	3	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	3	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	3	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	3	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	3	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	3	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	3	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	3	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	3	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	3	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	3	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	3	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	3	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	3	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	3	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	3	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	3	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	3	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	3	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	3	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	3	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	3	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	3	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	3	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	3	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	3	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	3	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	10	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	10	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	10	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	10	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	10	0.12
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	10	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	10	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	10	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	10	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	10	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	10	0.12
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	10	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	10	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	10	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	10	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	10	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	10	0.12
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	10	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	10	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	10	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	10	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	10	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	10	0.12
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	10	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	10	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	10	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	10	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	10	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	10	0.12
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	10	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	10	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	10	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	10	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	10	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	10	0.12
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	10	0.12
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG2	14	0.12
(1,2457)	1:56:B:PRO:HD2	1:67:B:MET:HG3	14	0.12
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG2	14	0.12
(1,2457)	1:56:B:PRO:HD3	1:67:B:MET:HG3	14	0.12
(1,2348)	1:42:B:PRO:HB2	1:45:B:LEU:HG	2	0.12
(1,2348)	1:42:B:PRO:HB3	1:45:B:LEU:HG	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB2	10	0.12
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB3	10	0.12
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB2	10	0.12
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB3	10	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB2	1	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB3	1	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB2	1	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB3	1	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB2	5	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB3	5	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB2	5	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB3	5	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB2	6	0.12
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB3	6	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB2	6	0.12
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB3	6	0.12
(1,2275)	1:24:B:VAL:HG11	1:36:B:LEU:HG	7	0.12
(1,2275)	1:24:B:VAL:HG12	1:36:B:LEU:HG	7	0.12
(1,2275)	1:24:B:VAL:HG13	1:36:B:LEU:HG	7	0.12
(1,2275)	1:24:B:VAL:HG21	1:36:B:LEU:HG	7	0.12
(1,2275)	1:24:B:VAL:HG22	1:36:B:LEU:HG	7	0.12
(1,2275)	1:24:B:VAL:HG23	1:36:B:LEU:HG	7	0.12
(1,2275)	1:24:B:VAL:HG11	1:36:B:LEU:HG	9	0.12
(1,2275)	1:24:B:VAL:HG12	1:36:B:LEU:HG	9	0.12
(1,2275)	1:24:B:VAL:HG13	1:36:B:LEU:HG	9	0.12
(1,2275)	1:24:B:VAL:HG21	1:36:B:LEU:HG	9	0.12
(1,2275)	1:24:B:VAL:HG22	1:36:B:LEU:HG	9	0.12
(1,2275)	1:24:B:VAL:HG23	1:36:B:LEU:HG	9	0.12
(1,2275)	1:24:B:VAL:HG11	1:36:B:LEU:HG	13	0.12
(1,2275)	1:24:B:VAL:HG12	1:36:B:LEU:HG	13	0.12
(1,2275)	1:24:B:VAL:HG13	1:36:B:LEU:HG	13	0.12
(1,2275)	1:24:B:VAL:HG21	1:36:B:LEU:HG	13	0.12
(1,2275)	1:24:B:VAL:HG22	1:36:B:LEU:HG	13	0.12
(1,2275)	1:24:B:VAL:HG23	1:36:B:LEU:HG	13	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	8	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	8	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	8	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	8	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	8	0.12
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	8	0.12
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	8	0.12
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	8	0.12
(1,2052)	1:98:B:ILE:HD11	1:24:B:VAL:HA	20	0.12
(1,2052)	1:98:B:ILE:HD12	1:24:B:VAL:HA	20	0.12
(1,2052)	1:98:B:ILE:HD13	1:24:B:VAL:HA	20	0.12
(1,2034)	1:91:B:ARG:HB2	1:95:B:ILE:HG13	6	0.12
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	7	0.12
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	7	0.12
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	13	0.12
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	13	0.12
(1,1978)	1:89:B:THR:HG1	1:90:B:PHE:HB2	14	0.12
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	4	0.12
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	4	0.12
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	4	0.12
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	4	0.12
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	4	0.12
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	4	0.12
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	4	0.12
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	4	0.12
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	4	0.12
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	4	0.12
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	4	0.12
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	4	0.12
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	13	0.12
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	13	0.12
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	13	0.12
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	13	0.12
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	13	0.12
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	13	0.12
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	13	0.12
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	13	0.12
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	13	0.12
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	13	0.12
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	13	0.12
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	13	0.12
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	18	0.12
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	1	0.12
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	1	0.12
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	1	0.12
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	1	0.12
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	1	0.12
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	1	0.12
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	4	0.12
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	4	0.12
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	4	0.12
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	4	0.12
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	4	0.12
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD23	6	0.12
(1,1947)	1:60:B:ILE:HG21	1:87:B:LEU:HD21	10	0.12
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	10	0.12
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	10	0.12
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	18	0.12
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	18	0.12
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG2	19	0.12
(1,1908)	1:84:B:VAL:HA	1:12:B:LYS:HG3	19	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	4	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	4	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	4	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	4	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	4	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	4	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	4	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	4	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	4	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	4	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	4	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	4	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	7	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	7	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	7	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	7	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	7	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	7	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	7	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	7	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	7	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	7	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	7	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	7	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	20	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	20	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	20	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	20	0.12
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	20	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	20	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	20	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	20	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	20	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	20	0.12
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	20	0.12
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	5	0.12
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	5	0.12
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	7	0.12
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	7	0.12
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	12	0.12
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	12	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	3	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	3	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	8	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	8	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	15	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	15	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	16	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	16	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	18	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	18	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG2	19	0.12
(1,1851)	1:78:B:LYS:HA	1:78:B:LYS:HG3	19	0.12
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	7	0.12
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	7	0.12
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	9	0.12
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	9	0.12
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	17	0.12
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	17	0.12
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	19	0.12
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	19	0.12
(1,1828)	1:34:B:THR:HG22	1:76:B:PRO:HG3	1	0.12
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	10	0.12
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	10	0.12
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	10	0.12
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	10	0.12
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	10	0.12
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	10	0.12
(1,1804)	1:73:B:THR:HG1	1:39:B:PRO:HG3	14	0.12
(1,1803)	1:39:B:PRO:HG3	1:73:B:THR:HG21	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1801)	1:37:B:VAL:HG23	1:73:B:THR:HG22	5	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	3	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	3	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	9	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	9	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	17	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	17	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	20	0.12
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	20	0.12
(1,1789)	1:40:B:LEU:HG	1:68:B:LEU:H	10	0.12
(1,1776)	1:67:B:MET:HG2	1:21:B:PHE:HA	7	0.12
(1,1776)	1:67:B:MET:HG3	1:21:B:PHE:HA	7	0.12
(1,1763)	1:42:B:PRO:HA	1:66:B:ILE:HG13	13	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD1	12	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD2	12	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD1	14	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD2	14	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD1	16	0.12
(1,1746)	1:43:B:ILE:HB	1:65:B:PHE:HD2	16	0.12
(1,1727)	1:58:B:ILE:HB	1:64:B:ASP:HA	5	0.12
(1,1727)	1:58:B:ILE:HB	1:64:B:ASP:HA	8	0.12
(1,1720)	1:43:B:ILE:HG13	1:64:B:ASP:HB2	1	0.12
(1,1711)	1:60:B:ILE:HG12	1:58:B:ILE:HD12	19	0.12
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	2	0.12
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	7	0.12
(1,1646)	1:43:B:ILE:HD11	1:43:B:ILE:HB	10	0.12
(1,1646)	1:43:B:ILE:HD12	1:43:B:ILE:HB	10	0.12
(1,1646)	1:43:B:ILE:HD13	1:43:B:ILE:HB	10	0.12
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	14	0.12
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	14	0.12
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	14	0.12
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	14	0.12
(1,1623)	1:39:B:PRO:HB2	1:40:B:LEU:HA	1	0.12
(1,1623)	1:39:B:PRO:HB3	1:40:B:LEU:HA	1	0.12
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	5	0.12
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	5	0.12
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	5	0.12
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	5	0.12
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	5	0.12
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	5	0.12
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	5	0.12
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	5	0.12
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	5	0.12
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	5	0.12
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	5	0.12
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	7	0.12
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	7	0.12
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	7	0.12
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	7	0.12
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	7	0.12
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	7	0.12
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	7	0.12
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	7	0.12
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	7	0.12
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	7	0.12
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	7	0.12
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	7	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB2	1	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB3	1	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB2	1	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB3	1	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB2	5	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB3	5	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB2	5	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB3	5	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB2	6	0.12
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB3	6	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB2	6	0.12
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB3	6	0.12
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB2	17	0.12
(1,1553)	1:26:B:SER:HA	1:29:B:LEU:HB3	17	0.12
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	4	0.12
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	7	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	1	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	1	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	1	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	1	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	1	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	1	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	2	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	2	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	2	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	2	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	2	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	5	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	5	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	5	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	5	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	5	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	5	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	6	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	6	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	6	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	6	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	6	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	6	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	9	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	9	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	9	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	9	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	9	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	9	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	16	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	16	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	16	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	16	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	16	0.12
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	16	0.12
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	2	0.12
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	2	0.12
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	3	0.12
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	3	0.12
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	11	0.12
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	11	0.12
(1,1450)	1:17:B:THR:HG1	1:16:B:LYS:HB2	12	0.12
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	19	0.12
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	19	0.12
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	8	0.12
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	8	0.12
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	10	0.12
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	10	0.12
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	20	0.12
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	20	0.12
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	1	0.12
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	3	0.12
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	3	0.12
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	8	0.12
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	8	0.12
(1,1380)	1:103:A:THR:HG1	1:105:A:ILE:HB	11	0.12
(1,1374)	1:103:A:THR:HG21	1:102:A:ILE:HG23	1	0.12
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	4	0.12
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	4	0.12
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	4	0.12
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	4	0.12
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	4	0.12
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	4	0.12
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	4	0.12
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	4	0.12
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	4	0.12
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	4	0.12
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	4	0.12
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	4	0.12
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	14	0.12
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	14	0.12
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	14	0.12
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	14	0.12
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	14	0.12
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	14	0.12
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	14	0.12
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	14	0.12
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	14	0.12
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	14	0.12
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	14	0.12
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	14	0.12
(1,1157)	1:79:A:ILE:HD11	1:75:A:VAL:HB	9	0.12
(1,1157)	1:79:A:ILE:HD12	1:75:A:VAL:HB	9	0.12
(1,1157)	1:79:A:ILE:HD13	1:75:A:VAL:HB	9	0.12
(1,1073)	1:56:A:PRO:HD2	1:67:A:MET:HG2	17	0.12
(1,1073)	1:56:A:PRO:HD2	1:67:A:MET:HG3	17	0.12
(1,1073)	1:56:A:PRO:HD3	1:67:A:MET:HG2	17	0.12
(1,1073)	1:56:A:PRO:HD3	1:67:A:MET:HG3	17	0.12
(1,964)	1:42:A:PRO:HB2	1:45:A:LEU:HG	4	0.12
(1,964)	1:42:A:PRO:HB3	1:45:A:LEU:HG	4	0.12
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	18	0.12
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	18	0.12
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	18	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	1	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	1	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	1	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	1	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	6	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	6	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	6	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	6	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	8	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	8	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	8	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	8	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	13	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	13	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	13	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	13	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	14	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	14	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	14	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	14	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	16	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	16	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	16	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	16	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	19	0.12
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	19	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	19	0.12
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	19	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD11	1	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD12	1	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD13	1	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD21	1	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD22	1	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD23	1	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD11	5	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD12	5	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD13	5	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD21	5	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD22	5	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD23	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD11	10	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD12	10	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD13	10	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD21	10	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD22	10	0.12
(1,725)	1:102:A:ILE:HA	1:101:A:LEU:HD23	10	0.12
(1,689)	1:69:A:THR:HG1	1:100:A:PHE:HD2	20	0.12
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	4	0.12
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	10	0.12
(1,669)	1:69:A:THR:HG21	1:98:A:ILE:H	11	0.12
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	9	0.12
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	9	0.12
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	9	0.12
(1,650)	1:91:A:ARG:HB2	1:95:A:ILE:HG13	4	0.12
(1,650)	1:91:A:ARG:HB2	1:95:A:ILE:HG13	18	0.12
(1,641)	1:94:A:ILE:HG13	1:22:A:VAL:HB	7	0.12
(1,641)	1:94:A:ILE:HG13	1:22:A:VAL:HB	8	0.12
(1,640)	1:94:A:ILE:HA	1:22:A:VAL:HG11	2	0.12
(1,640)	1:94:A:ILE:HA	1:22:A:VAL:HG12	2	0.12
(1,640)	1:94:A:ILE:HA	1:22:A:VAL:HG13	2	0.12
(1,640)	1:94:A:ILE:HA	1:22:A:VAL:HG21	2	0.12
(1,640)	1:94:A:ILE:HA	1:22:A:VAL:HG22	2	0.12
(1,640)	1:94:A:ILE:HA	1:22:A:VAL:HG23	2	0.12
(1,639)	1:94:A:ILE:HG21	1:4:A:PHE:HE1	10	0.12
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	8	0.12
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	8	0.12
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	20	0.12
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	20	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	2	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	2	0.12
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	2	0.12
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	2	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	2	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	2	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	2	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	2	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	2	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	2	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	2	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	2	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	6	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	6	0.12
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	6	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	6	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	6	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	6	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	6	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	6	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	6	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	6	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	6	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	11	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	11	0.12
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	11	0.12
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	11	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	11	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	11	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	11	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	11	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	11	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	11	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	11	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	11	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	20	0.12
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	20	0.12
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	20	0.12
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	20	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	20	0.12
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	20	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	20	0.12
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	20	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	20	0.12
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	20	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	20	0.12
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	20	0.12
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	15	0.12
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	15	0.12
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	15	0.12
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	15	0.12
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	15	0.12
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	15	0.12
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	20	0.12
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	20	0.12
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	20	0.12
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	20	0.12
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	20	0.12
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	11	0.12
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	11	0.12
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	16	0.12
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	16	0.12
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	10	0.12
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	10	0.12
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	10	0.12
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	10	0.12
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	10	0.12
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	10	0.12
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	10	0.12
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	10	0.12
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	10	0.12
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	10	0.12
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	10	0.12
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	10	0.12
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB2	13	0.12
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB3	13	0.12
(1,478)	1:79:A:ILE:HD11	1:79:A:ILE:HA	14	0.12
(1,478)	1:79:A:ILE:HD12	1:79:A:ILE:HA	14	0.12
(1,478)	1:79:A:ILE:HD13	1:79:A:ILE:HA	14	0.12
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	11	0.12
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	11	0.12
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG11	19	0.12
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG12	19	0.12
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG13	19	0.12
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG21	19	0.12
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG22	19	0.12
(1,472)	1:79:A:ILE:HD11	1:75:A:VAL:HG23	19	0.12
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG11	19	0.12
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG12	19	0.12
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG13	19	0.12
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG21	19	0.12
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG22	19	0.12
(1,472)	1:79:A:ILE:HD12	1:75:A:VAL:HG23	19	0.12
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG11	19	0.12
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG12	19	0.12
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG13	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG21	19	0.12
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG22	19	0.12
(1,472)	1:79:A:ILE:HD13	1:75:A:VAL:HG23	19	0.12
(1,471)	1:79:A:ILE:HD11	1:75:A:VAL:HA	18	0.12
(1,471)	1:79:A:ILE:HD12	1:75:A:VAL:HA	18	0.12
(1,471)	1:79:A:ILE:HD13	1:75:A:VAL:HA	18	0.12
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD1	7	0.12
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD2	7	0.12
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD1	7	0.12
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD2	7	0.12
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD1	7	0.12
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD2	7	0.12
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD1	15	0.12
(1,470)	1:79:A:ILE:HD11	1:21:A:PHE:HD2	15	0.12
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD1	15	0.12
(1,470)	1:79:A:ILE:HD12	1:21:A:PHE:HD2	15	0.12
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD1	15	0.12
(1,470)	1:79:A:ILE:HD13	1:21:A:PHE:HD2	15	0.12
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	13	0.12
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	13	0.12
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	20	0.12
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	20	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	4	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	4	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	5	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	5	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	6	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	6	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	7	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	7	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	9	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	9	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	11	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	11	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	14	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	14	0.12
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	20	0.12
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	20	0.12
(1,410)	1:69:A:THR:HG1	1:56:A:PRO:HD3	13	0.12
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	6	0.12
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	10	0.12
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	13	0.12
(1,383)	1:56:A:PRO:HA	1:66:A:ILE:HG21	10	0.12
(1,354)	1:42:A:PRO:HB2	1:65:A:PHE:HA	6	0.12
(1,354)	1:42:A:PRO:HB3	1:65:A:PHE:HA	6	0.12
(1,321)	1:59:A:HIS:HB2	1:57:A:THR:HG23	16	0.12
(1,320)	1:58:A:ILE:HB	1:58:A:ILE:H	19	0.12
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	1	0.12
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	10	0.12
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	15	0.12
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	17	0.12
(1,279)	1:43:A:ILE:HG21	1:48:A:LYS:HG2	6	0.12
(1,278)	1:48:A:LYS:HD2	1:43:A:ILE:HG21	13	0.12
(1,251)	1:19:A:PRO:HG2	1:41:A:THR:HB	5	0.12
(1,251)	1:19:A:PRO:HG3	1:41:A:THR:HB	5	0.12
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	18	0.12
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	18	0.12
(1,237)	1:40:A:LEU:HD11	1:20:A:TYR:HE1	19	0.12
(1,237)	1:40:A:LEU:HD11	1:20:A:TYR:HE2	19	0.12
(1,237)	1:40:A:LEU:HD12	1:20:A:TYR:HE1	19	0.12
(1,237)	1:40:A:LEU:HD12	1:20:A:TYR:HE2	19	0.12
(1,237)	1:40:A:LEU:HD13	1:20:A:TYR:HE1	19	0.12
(1,237)	1:40:A:LEU:HD13	1:20:A:TYR:HE2	19	0.12
(1,237)	1:40:A:LEU:HD21	1:20:A:TYR:HE1	19	0.12
(1,237)	1:40:A:LEU:HD21	1:20:A:TYR:HE2	19	0.12
(1,237)	1:40:A:LEU:HD22	1:20:A:TYR:HE1	19	0.12
(1,237)	1:40:A:LEU:HD22	1:20:A:TYR:HE2	19	0.12
(1,237)	1:40:A:LEU:HD23	1:20:A:TYR:HE1	19	0.12
(1,237)	1:40:A:LEU:HD23	1:20:A:TYR:HE2	19	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	8	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	8	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	8	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	8	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	8	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	8	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	8	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	8	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	8	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	8	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	8	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	8	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	11	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	11	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	11	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	11	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	11	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	11	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	11	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	11	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	11	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	11	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	11	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	12	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	12	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	12	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	12	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	12	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	12	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	12	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	12	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	12	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	12	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	12	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	12	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	15	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	15	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	15	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	15	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	15	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	15	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	15	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	15	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	15	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	15	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	15	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	15	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	17	0.12
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	17	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	17	0.12
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	17	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	17	0.12
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	17	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	17	0.12
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	17	0.12
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	17	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	17	0.12
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	17	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	1	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	1	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	1	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	1	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	6	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	6	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	6	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	6	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	8	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	8	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	8	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	8	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	13	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	13	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	13	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	13	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	14	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	14	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	14	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	14	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	16	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	16	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	16	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	16	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	19	0.12
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	19	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	19	0.12
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	19	0.12
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG23	6	0.12
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG22	10	0.12
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	6	0.12
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	11	0.12
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	13	0.12
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	14	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG11	8	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG12	8	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG13	8	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG21	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG22	8	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG23	8	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG11	13	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG12	13	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG13	13	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG21	13	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG22	13	0.12
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG23	13	0.12
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	3	0.12
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	3	0.12
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	13	0.12
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	13	0.12
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	14	0.12
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	14	0.12
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	3	0.12
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	3	0.12
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD2	15	0.12
(1,48)	1:11:A:ASP:HA	1:10:A:LYS:HD3	15	0.12
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	4	0.12
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	4	0.12
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	8	0.12
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	8	0.12
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	13	0.12
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	13	0.12
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	18	0.12
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	18	0.12
(1,3290)	1:71:A:GLN:HA	1:74:B:SER:HA	8	0.11
(1,3141)	1:26:B:SER:H	1:25:B:GLN:HA	2	0.11
(1,3141)	1:26:B:SER:H	1:25:B:GLN:HA	10	0.11
(1,3141)	1:26:B:SER:H	1:25:B:GLN:HA	20	0.11
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG2	10	0.11
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG3	10	0.11
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG2	18	0.11
(1,3134)	1:20:B:TYR:H	1:19:B:PRO:HG3	18	0.11
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	4	0.11
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	14	0.11
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	15	0.11
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	8	0.11
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	14	0.11
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	16	0.11
(1,3092)	1:103:B:THR:H	1:100:B:PHE:H	20	0.11
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3089)	1:96:B:ALA:H	1:92:B:ASN:HB3	10	0.11
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	9	0.11
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	15	0.11
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	19	0.11
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB2	7	0.11
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB3	7	0.11
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	1	0.11
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	9	0.11
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	10	0.11
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	14	0.11
(1,3052)	1:36:B:LEU:H	1:26:B:SER:H	19	0.11
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	18	0.11
(1,3045)	1:30:B:ASP:H	1:29:B:LEU:HB2	10	0.11
(1,3045)	1:30:B:ASP:H	1:29:B:LEU:HB3	10	0.11
(1,2906)	1:40:A:LEU:H	1:40:A:LEU:HB2	2	0.11
(1,2906)	1:40:A:LEU:H	1:40:A:LEU:HB3	2	0.11
(1,2906)	1:40:A:LEU:H	1:40:A:LEU:HB2	16	0.11
(1,2906)	1:40:A:LEU:H	1:40:A:LEU:HB3	16	0.11
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	3	0.11
(1,2883)	1:26:A:SER:H	1:25:A:GLN:HA	20	0.11
(1,2845)	1:9:A:ASN:H	1:8:A:LYS:HA	8	0.11
(1,2845)	1:9:A:ASN:H	1:8:A:LYS:HA	12	0.11
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	11	0.11
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	14	0.11
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	15	0.11
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB2	4	0.11
(1,2832)	1:100:A:PHE:H	1:101:A:LEU:HB3	4	0.11
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB2	16	0.11
(1,2831)	1:96:A:ALA:H	1:92:A:ASN:HB3	16	0.11
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	4	0.11
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	6	0.11
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	12	0.11
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	13	0.11
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	18	0.11
(1,2828)	1:88:A:SER:H	1:90:A:PHE:H	19	0.11
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	2	0.11
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	6	0.11
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	9	0.11
(1,2812)	1:57:A:THR:H	1:66:A:ILE:HG21	13	0.11
(1,2811)	1:66:A:ILE:H	1:43:A:ILE:HG13	3	0.11
(1,2809)	1:66:A:ILE:H	1:40:A:LEU:HA	5	0.11
(1,2807)	1:63:A:GLY:H	1:60:A:ILE:HG21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	12	0.11
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	13	0.11
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	8	0.11
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	12	0.11
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	16	0.11
(1,2792)	1:36:A:LEU:H	1:24:A:VAL:H	2	0.11
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	13	0.11
(1,2767)	1:105:B:ILE:HD11	1:105:B:ILE:HA	6	0.11
(1,2767)	1:105:B:ILE:HD12	1:105:B:ILE:HA	6	0.11
(1,2767)	1:105:B:ILE:HD13	1:105:B:ILE:HA	6	0.11
(1,2767)	1:105:B:ILE:HD11	1:105:B:ILE:HA	9	0.11
(1,2767)	1:105:B:ILE:HD12	1:105:B:ILE:HA	9	0.11
(1,2767)	1:105:B:ILE:HD13	1:105:B:ILE:HA	9	0.11
(1,2620)	1:87:B:LEU:HD11	1:58:B:ILE:HD11	20	0.11
(1,2620)	1:87:B:LEU:HD11	1:58:B:ILE:HD12	20	0.11
(1,2620)	1:87:B:LEU:HD11	1:58:B:ILE:HD13	20	0.11
(1,2620)	1:87:B:LEU:HD12	1:58:B:ILE:HD11	20	0.11
(1,2620)	1:87:B:LEU:HD12	1:58:B:ILE:HD12	20	0.11
(1,2620)	1:87:B:LEU:HD12	1:58:B:ILE:HD13	20	0.11
(1,2620)	1:87:B:LEU:HD13	1:58:B:ILE:HD11	20	0.11
(1,2620)	1:87:B:LEU:HD13	1:58:B:ILE:HD12	20	0.11
(1,2620)	1:87:B:LEU:HD13	1:58:B:ILE:HD13	20	0.11
(1,2620)	1:87:B:LEU:HD21	1:58:B:ILE:HD11	20	0.11
(1,2620)	1:87:B:LEU:HD21	1:58:B:ILE:HD12	20	0.11
(1,2620)	1:87:B:LEU:HD21	1:58:B:ILE:HD13	20	0.11
(1,2620)	1:87:B:LEU:HD22	1:58:B:ILE:HD11	20	0.11
(1,2620)	1:87:B:LEU:HD22	1:58:B:ILE:HD12	20	0.11
(1,2620)	1:87:B:LEU:HD22	1:58:B:ILE:HD13	20	0.11
(1,2620)	1:87:B:LEU:HD23	1:58:B:ILE:HD11	20	0.11
(1,2620)	1:87:B:LEU:HD23	1:58:B:ILE:HD12	20	0.11
(1,2620)	1:87:B:LEU:HD23	1:58:B:ILE:HD13	20	0.11
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB2	10	0.11
(1,2618)	1:22:B:VAL:HG11	1:87:B:LEU:HB3	10	0.11
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB2	10	0.11
(1,2618)	1:22:B:VAL:HG12	1:87:B:LEU:HB3	10	0.11
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB2	10	0.11
(1,2618)	1:22:B:VAL:HG13	1:87:B:LEU:HB3	10	0.11
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB2	10	0.11
(1,2618)	1:22:B:VAL:HG21	1:87:B:LEU:HB3	10	0.11
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB2	10	0.11
(1,2618)	1:22:B:VAL:HG22	1:87:B:LEU:HB3	10	0.11
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2618)	1:22:B:VAL:HG23	1:87:B:LEU:HB3	10	0.11
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	17	0.11
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	17	0.11
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	17	0.11
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG11	18	0.11
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG12	18	0.11
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG13	18	0.11
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG21	18	0.11
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG22	18	0.11
(1,2499)	1:75:B:VAL:HG11	1:37:B:VAL:HG23	18	0.11
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG11	18	0.11
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG12	18	0.11
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG13	18	0.11
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG21	18	0.11
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG22	18	0.11
(1,2499)	1:75:B:VAL:HG12	1:37:B:VAL:HG23	18	0.11
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG11	18	0.11
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG12	18	0.11
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG13	18	0.11
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG21	18	0.11
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG22	18	0.11
(1,2499)	1:75:B:VAL:HG13	1:37:B:VAL:HG23	18	0.11
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG11	18	0.11
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG12	18	0.11
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG13	18	0.11
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG21	18	0.11
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG22	18	0.11
(1,2499)	1:75:B:VAL:HG21	1:37:B:VAL:HG23	18	0.11
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG11	18	0.11
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG12	18	0.11
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG13	18	0.11
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG21	18	0.11
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG22	18	0.11
(1,2499)	1:75:B:VAL:HG22	1:37:B:VAL:HG23	18	0.11
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG11	18	0.11
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG12	18	0.11
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG13	18	0.11
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG21	18	0.11
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG22	18	0.11
(1,2499)	1:75:B:VAL:HG23	1:37:B:VAL:HG23	18	0.11
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB2	4	0.11
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB2	4	0.11
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB3	4	0.11
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB2	5	0.11
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB3	5	0.11
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB2	5	0.11
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB3	5	0.11
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB2	9	0.11
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB3	9	0.11
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB2	9	0.11
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB3	9	0.11
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB2	16	0.11
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB3	16	0.11
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB2	16	0.11
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB3	16	0.11
(1,2275)	1:24:B:VAL:HG11	1:36:B:LEU:HG	1	0.11
(1,2275)	1:24:B:VAL:HG12	1:36:B:LEU:HG	1	0.11
(1,2275)	1:24:B:VAL:HG13	1:36:B:LEU:HG	1	0.11
(1,2275)	1:24:B:VAL:HG21	1:36:B:LEU:HG	1	0.11
(1,2275)	1:24:B:VAL:HG22	1:36:B:LEU:HG	1	0.11
(1,2275)	1:24:B:VAL:HG23	1:36:B:LEU:HG	1	0.11
(1,2275)	1:24:B:VAL:HG11	1:36:B:LEU:HG	16	0.11
(1,2275)	1:24:B:VAL:HG12	1:36:B:LEU:HG	16	0.11
(1,2275)	1:24:B:VAL:HG13	1:36:B:LEU:HG	16	0.11
(1,2275)	1:24:B:VAL:HG21	1:36:B:LEU:HG	16	0.11
(1,2275)	1:24:B:VAL:HG22	1:36:B:LEU:HG	16	0.11
(1,2275)	1:24:B:VAL:HG23	1:36:B:LEU:HG	16	0.11
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	11	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	3	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	3	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	3	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	3	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	3	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	3	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	20	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	20	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	20	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	20	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	20	0.11
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	20	0.11
(1,2108)	1:99:B:ASP:HA	1:102:B:ILE:H	10	0.11
(1,2062)	1:96:B:ALA:HA	1:99:B:ASP:HA	1	0.11
(1,2053)	1:69:B:THR:HG23	1:98:B:ILE:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2034)	1:91:B:ARG:HB2	1:95:B:ILE:HG13	1	0.11
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	7	0.11
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	13	0.11
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	20	0.11
(1,2023)	1:94:B:ILE:HG13	1:4:B:PHE:HE1	10	0.11
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	8	0.11
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	8	0.11
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE1	9	0.11
(1,1977)	1:87:B:LEU:HD11	1:90:B:PHE:HE2	9	0.11
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE1	9	0.11
(1,1977)	1:87:B:LEU:HD12	1:90:B:PHE:HE2	9	0.11
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE1	9	0.11
(1,1977)	1:87:B:LEU:HD13	1:90:B:PHE:HE2	9	0.11
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE1	9	0.11
(1,1977)	1:87:B:LEU:HD21	1:90:B:PHE:HE2	9	0.11
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE1	9	0.11
(1,1977)	1:87:B:LEU:HD22	1:90:B:PHE:HE2	9	0.11
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE1	9	0.11
(1,1977)	1:87:B:LEU:HD23	1:90:B:PHE:HE2	9	0.11
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	7	0.11
(1,1961)	1:90:B:PHE:HE1	1:57:B:THR:HB	6	0.11
(1,1961)	1:90:B:PHE:HE2	1:57:B:THR:HB	6	0.11
(1,1959)	1:89:B:THR:HG22	1:87:B:LEU:HB2	19	0.11
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	5	0.11
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	5	0.11
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	5	0.11
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	5	0.11
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	5	0.11
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	5	0.11
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	15	0.11
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	15	0.11
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	15	0.11
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	15	0.11
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	15	0.11
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	15	0.11
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD1	2	0.11
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD2	2	0.11
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD1	2	0.11
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD2	2	0.11
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD1	2	0.11
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD2	2	0.11
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD1	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD2	2	0.11
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD1	2	0.11
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD2	2	0.11
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD1	2	0.11
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD2	2	0.11
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB2	2	0.11
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB3	2	0.11
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB2	13	0.11
(1,1868)	1:80:B:LEU:HA	1:7:B:TYR:HB3	13	0.11
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	18	0.11
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	18	0.11
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	18	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	3	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	3	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	4	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	4	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	6	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	6	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	8	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	8	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB2	15	0.11
(1,1858)	1:79:B:ILE:HA	1:78:B:LYS:HB3	15	0.11
(1,1854)	1:79:B:ILE:HD11	1:21:B:PHE:HD1	10	0.11
(1,1854)	1:79:B:ILE:HD11	1:21:B:PHE:HD2	10	0.11
(1,1854)	1:79:B:ILE:HD12	1:21:B:PHE:HD1	10	0.11
(1,1854)	1:79:B:ILE:HD12	1:21:B:PHE:HD2	10	0.11
(1,1854)	1:79:B:ILE:HD13	1:21:B:PHE:HD1	10	0.11
(1,1854)	1:79:B:ILE:HD13	1:21:B:PHE:HD2	10	0.11
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	1	0.11
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	1	0.11
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	11	0.11
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	11	0.11
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	14	0.11
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	14	0.11
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	16	0.11
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	16	0.11
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	18	0.11
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	18	0.11
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	20	0.11
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	20	0.11
(1,1829)	1:76:B:PRO:HG3	1:34:B:THR:HG23	4	0.11
(1,1804)	1:73:B:THR:HG1	1:39:B:PRO:HG3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1804)	1:73:B:THR:HG1	1:39:B:PRO:HG3	11	0.11
(1,1804)	1:73:B:THR:HG23	1:39:B:PRO:HG3	12	0.11
(1,1801)	1:37:B:VAL:HG22	1:73:B:THR:HG23	6	0.11
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	8	0.11
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	8	0.11
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	10	0.11
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	10	0.11
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB2	19	0.11
(1,1790)	1:41:B:THR:HB	1:68:B:LEU:HB3	19	0.11
(1,1789)	1:40:B:LEU:HG	1:68:B:LEU:H	2	0.11
(1,1789)	1:40:B:LEU:HG	1:68:B:LEU:H	5	0.11
(1,1789)	1:40:B:LEU:HG	1:68:B:LEU:H	6	0.11
(1,1765)	1:66:B:ILE:HG13	1:43:B:ILE:HG21	14	0.11
(1,1763)	1:42:B:PRO:HA	1:66:B:ILE:HG13	16	0.11
(1,1745)	1:43:B:ILE:HG12	1:65:B:PHE:HB3	15	0.11
(1,1731)	1:19:B:PRO:HG2	1:65:B:PHE:HD1	11	0.11
(1,1731)	1:19:B:PRO:HG2	1:65:B:PHE:HD2	11	0.11
(1,1731)	1:19:B:PRO:HG3	1:65:B:PHE:HD1	11	0.11
(1,1731)	1:19:B:PRO:HG3	1:65:B:PHE:HD2	11	0.11
(1,1727)	1:58:B:ILE:HB	1:64:B:ASP:HA	2	0.11
(1,1727)	1:58:B:ILE:HB	1:64:B:ASP:HA	19	0.11
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	9	0.11
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	18	0.11
(1,1666)	1:47:B:ASP:HB2	1:48:B:LYS:HA	11	0.11
(1,1666)	1:47:B:ASP:HB3	1:48:B:LYS:HA	11	0.11
(1,1666)	1:47:B:ASP:HB2	1:48:B:LYS:HA	12	0.11
(1,1666)	1:47:B:ASP:HB3	1:48:B:LYS:HA	12	0.11
(1,1666)	1:47:B:ASP:HB2	1:48:B:LYS:HA	16	0.11
(1,1666)	1:47:B:ASP:HB3	1:48:B:LYS:HA	16	0.11
(1,1666)	1:47:B:ASP:HB2	1:48:B:LYS:HA	20	0.11
(1,1666)	1:47:B:ASP:HB3	1:48:B:LYS:HA	20	0.11
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	6	0.11
(1,1647)	1:43:B:ILE:HB	1:43:B:ILE:HG13	10	0.11
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB2	16	0.11
(1,1643)	1:19:B:PRO:HG2	1:42:B:PRO:HB3	16	0.11
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB2	16	0.11
(1,1643)	1:19:B:PRO:HG3	1:42:B:PRO:HB3	16	0.11
(1,1635)	1:19:B:PRO:HG2	1:41:B:THR:HB	2	0.11
(1,1635)	1:19:B:PRO:HG3	1:41:B:THR:HB	2	0.11
(1,1635)	1:19:B:PRO:HG2	1:41:B:THR:HB	13	0.11
(1,1635)	1:19:B:PRO:HG3	1:41:B:THR:HB	13	0.11
(1,1635)	1:19:B:PRO:HG2	1:41:B:THR:HB	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:19:B:PRO:HG3	1:41:B:THR:HB	16	0.11
(1,1634)	1:41:B:THR:HB	1:17:B:THR:HG23	16	0.11
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	6	0.11
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	6	0.11
(1,1623)	1:39:B:PRO:HB2	1:40:B:LEU:HA	8	0.11
(1,1623)	1:39:B:PRO:HB3	1:40:B:LEU:HA	8	0.11
(1,1623)	1:39:B:PRO:HB2	1:40:B:LEU:HA	16	0.11
(1,1623)	1:39:B:PRO:HB3	1:40:B:LEU:HA	16	0.11
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	14	0.11
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	14	0.11
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	14	0.11
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	14	0.11
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	14	0.11
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	14	0.11
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	14	0.11
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	14	0.11
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	14	0.11
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	14	0.11
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	14	0.11
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	14	0.11
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB2	9	0.11
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB3	9	0.11
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB2	9	0.11
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB3	9	0.11
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB2	16	0.11
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB3	16	0.11
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB2	16	0.11
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB3	16	0.11
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	1	0.11
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	8	0.11
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	16	0.11
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	19	0.11
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	13	0.11
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	13	0.11
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	13	0.11
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	13	0.11
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	13	0.11
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	13	0.11
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	8	0.11
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	8	0.11
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	9	0.11
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:17:B:THR:HG1	1:16:B:LYS:HB3	11	0.11
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	6	0.11
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	6	0.11
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	2	0.11
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	2	0.11
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	15	0.11
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	15	0.11
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	10	0.11
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	10	0.11
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	11	0.11
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	11	0.11
(1,1383)	1:105:A:ILE:HD11	1:105:A:ILE:HA	5	0.11
(1,1383)	1:105:A:ILE:HD12	1:105:A:ILE:HA	5	0.11
(1,1383)	1:105:A:ILE:HD13	1:105:A:ILE:HA	5	0.11
(1,1316)	1:95:A:ILE:HA	1:98:A:ILE:HD11	11	0.11
(1,1316)	1:95:A:ILE:HA	1:98:A:ILE:HD12	11	0.11
(1,1316)	1:95:A:ILE:HA	1:98:A:ILE:HD13	11	0.11
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD11	8	0.11
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD12	8	0.11
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD13	8	0.11
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD11	8	0.11
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD12	8	0.11
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD13	8	0.11
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD11	8	0.11
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD12	8	0.11
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD13	8	0.11
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD11	8	0.11
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD12	8	0.11
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD13	8	0.11
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD11	8	0.11
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD12	8	0.11
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD13	8	0.11
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD11	8	0.11
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD12	8	0.11
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD13	8	0.11
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB2	17	0.11
(1,1234)	1:22:A:VAL:HG11	1:87:A:LEU:HB3	17	0.11
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB2	17	0.11
(1,1234)	1:22:A:VAL:HG12	1:87:A:LEU:HB3	17	0.11
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB2	17	0.11
(1,1234)	1:22:A:VAL:HG13	1:87:A:LEU:HB3	17	0.11
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1234)	1:22:A:VAL:HG21	1:87:A:LEU:HB3	17	0.11
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB2	17	0.11
(1,1234)	1:22:A:VAL:HG22	1:87:A:LEU:HB3	17	0.11
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB2	17	0.11
(1,1234)	1:22:A:VAL:HG23	1:87:A:LEU:HB3	17	0.11
(1,1157)	1:79:A:ILE:HD11	1:75:A:VAL:HB	12	0.11
(1,1157)	1:79:A:ILE:HD12	1:75:A:VAL:HB	12	0.11
(1,1157)	1:79:A:ILE:HD13	1:75:A:VAL:HB	12	0.11
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG11	15	0.11
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG12	15	0.11
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG13	15	0.11
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG21	15	0.11
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG22	15	0.11
(1,1115)	1:75:A:VAL:HG11	1:37:A:VAL:HG23	15	0.11
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG11	15	0.11
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG12	15	0.11
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG13	15	0.11
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG21	15	0.11
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG22	15	0.11
(1,1115)	1:75:A:VAL:HG12	1:37:A:VAL:HG23	15	0.11
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG11	15	0.11
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG12	15	0.11
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG13	15	0.11
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG21	15	0.11
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG22	15	0.11
(1,1115)	1:75:A:VAL:HG13	1:37:A:VAL:HG23	15	0.11
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG11	15	0.11
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG12	15	0.11
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG13	15	0.11
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG21	15	0.11
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG22	15	0.11
(1,1115)	1:75:A:VAL:HG21	1:37:A:VAL:HG23	15	0.11
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG11	15	0.11
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG12	15	0.11
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG13	15	0.11
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG21	15	0.11
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG22	15	0.11
(1,1115)	1:75:A:VAL:HG22	1:37:A:VAL:HG23	15	0.11
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG11	15	0.11
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG12	15	0.11
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG13	15	0.11
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG22	15	0.11
(1,1115)	1:75:A:VAL:HG23	1:37:A:VAL:HG23	15	0.11
(1,1114)	1:75:A:VAL:HG11	1:35:A:ARG:HB2	18	0.11
(1,1114)	1:75:A:VAL:HG11	1:35:A:ARG:HB3	18	0.11
(1,1114)	1:75:A:VAL:HG12	1:35:A:ARG:HB2	18	0.11
(1,1114)	1:75:A:VAL:HG12	1:35:A:ARG:HB3	18	0.11
(1,1114)	1:75:A:VAL:HG13	1:35:A:ARG:HB2	18	0.11
(1,1114)	1:75:A:VAL:HG13	1:35:A:ARG:HB3	18	0.11
(1,1114)	1:75:A:VAL:HG21	1:35:A:ARG:HB2	18	0.11
(1,1114)	1:75:A:VAL:HG21	1:35:A:ARG:HB3	18	0.11
(1,1114)	1:75:A:VAL:HG22	1:35:A:ARG:HB2	18	0.11
(1,1114)	1:75:A:VAL:HG22	1:35:A:ARG:HB3	18	0.11
(1,1114)	1:75:A:VAL:HG23	1:35:A:ARG:HB2	18	0.11
(1,1114)	1:75:A:VAL:HG23	1:35:A:ARG:HB3	18	0.11
(1,1056)	1:66:A:ILE:HD11	1:66:A:ILE:HA	9	0.11
(1,1056)	1:66:A:ILE:HD12	1:66:A:ILE:HA	9	0.11
(1,1056)	1:66:A:ILE:HD13	1:66:A:ILE:HA	9	0.11
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	9	0.11
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	9	0.11
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	9	0.11
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	9	0.11
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	19	0.11
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	19	0.11
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	19	0.11
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	19	0.11
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB2	20	0.11
(1,959)	1:42:A:PRO:HB2	1:44:A:GLU:HB3	20	0.11
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB2	20	0.11
(1,959)	1:42:A:PRO:HB3	1:44:A:GLU:HB3	20	0.11
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB2	12	0.11
(1,892)	1:25:A:GLN:HB2	1:36:A:LEU:HB3	12	0.11
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB2	12	0.11
(1,892)	1:25:A:GLN:HB3	1:36:A:LEU:HB3	12	0.11
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	6	0.11
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	6	0.11
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	6	0.11
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	6	0.11
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	6	0.11
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	6	0.11
(1,724)	1:99:A:ASP:HA	1:102:A:ILE:H	10	0.11
(1,724)	1:99:A:ASP:HA	1:102:A:ILE:H	19	0.11
(1,708)	1:101:A:LEU:HD11	1:72:A:MET:HB2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:101:A:LEU:HD11	1:72:A:MET:HB3	19	0.11
(1,708)	1:101:A:LEU:HD12	1:72:A:MET:HB2	19	0.11
(1,708)	1:101:A:LEU:HD12	1:72:A:MET:HB3	19	0.11
(1,708)	1:101:A:LEU:HD13	1:72:A:MET:HB2	19	0.11
(1,708)	1:101:A:LEU:HD13	1:72:A:MET:HB3	19	0.11
(1,708)	1:101:A:LEU:HD21	1:72:A:MET:HB2	19	0.11
(1,708)	1:101:A:LEU:HD21	1:72:A:MET:HB3	19	0.11
(1,708)	1:101:A:LEU:HD22	1:72:A:MET:HB2	19	0.11
(1,708)	1:101:A:LEU:HD22	1:72:A:MET:HB3	19	0.11
(1,708)	1:101:A:LEU:HD23	1:72:A:MET:HB2	19	0.11
(1,708)	1:101:A:LEU:HD23	1:72:A:MET:HB3	19	0.11
(1,705)	1:101:A:LEU:HD11	1:69:A:THR:HB	16	0.11
(1,705)	1:101:A:LEU:HD12	1:69:A:THR:HB	16	0.11
(1,705)	1:101:A:LEU:HD13	1:69:A:THR:HB	16	0.11
(1,705)	1:101:A:LEU:HD21	1:69:A:THR:HB	16	0.11
(1,705)	1:101:A:LEU:HD22	1:69:A:THR:HB	16	0.11
(1,705)	1:101:A:LEU:HD23	1:69:A:THR:HB	16	0.11
(1,681)	1:96:A:ALA:HB1	1:99:A:ASP:HB2	17	0.11
(1,681)	1:96:A:ALA:HB1	1:99:A:ASP:HB3	17	0.11
(1,681)	1:96:A:ALA:HB2	1:99:A:ASP:HB2	17	0.11
(1,681)	1:96:A:ALA:HB2	1:99:A:ASP:HB3	17	0.11
(1,681)	1:96:A:ALA:HB3	1:99:A:ASP:HB2	17	0.11
(1,681)	1:96:A:ALA:HB3	1:99:A:ASP:HB3	17	0.11
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	16	0.11
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	7	0.11
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	7	0.11
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	7	0.11
(1,650)	1:91:A:ARG:HB2	1:95:A:ILE:HG13	16	0.11
(1,641)	1:94:A:ILE:HG13	1:22:A:VAL:HB	9	0.11
(1,641)	1:94:A:ILE:HG21	1:22:A:VAL:HB	11	0.11
(1,641)	1:94:A:ILE:HG21	1:22:A:VAL:HB	14	0.11
(1,639)	1:94:A:ILE:HG21	1:4:A:PHE:HE1	2	0.11
(1,626)	1:91:A:ARG:HG2	1:92:A:ASN:HA	5	0.11
(1,626)	1:91:A:ARG:HG3	1:92:A:ASN:HA	5	0.11
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	12	0.11
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	12	0.11
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	13	0.11
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	13	0.11
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	19	0.11
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	19	0.11
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	5	0.11
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	5	0.11
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	5	0.11
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	5	0.11
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	5	0.11
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	5	0.11
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	5	0.11
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	5	0.11
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	5	0.11
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	5	0.11
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	5	0.11
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE1	10	0.11
(1,593)	1:87:A:LEU:HD11	1:90:A:PHE:HE2	10	0.11
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE1	10	0.11
(1,593)	1:87:A:LEU:HD12	1:90:A:PHE:HE2	10	0.11
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE1	10	0.11
(1,593)	1:87:A:LEU:HD13	1:90:A:PHE:HE2	10	0.11
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE1	10	0.11
(1,593)	1:87:A:LEU:HD21	1:90:A:PHE:HE2	10	0.11
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE1	10	0.11
(1,593)	1:87:A:LEU:HD22	1:90:A:PHE:HE2	10	0.11
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE1	10	0.11
(1,593)	1:87:A:LEU:HD23	1:90:A:PHE:HE2	10	0.11
(1,585)	1:58:A:ILE:HB	1:90:A:PHE:HZ	5	0.11
(1,585)	1:58:A:ILE:HB	1:90:A:PHE:HZ	17	0.11
(1,575)	1:89:A:THR:HG23	1:87:A:LEU:HB2	16	0.11
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	8	0.11
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	8	0.11
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	8	0.11
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	8	0.11
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	8	0.11
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	8	0.11
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	11	0.11
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	11	0.11
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	11	0.11
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	11	0.11
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	11	0.11
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	11	0.11
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	13	0.11
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	13	0.11
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	13	0.11
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	13	0.11
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	13	0.11
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	14	0.11
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	14	0.11
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	14	0.11
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	14	0.11
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	14	0.11
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	14	0.11
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	16	0.11
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	16	0.11
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	16	0.11
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	16	0.11
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	16	0.11
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	16	0.11
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	18	0.11
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	18	0.11
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	18	0.11
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	18	0.11
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	18	0.11
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	18	0.11
(1,572)	1:87:A:LEU:HD11	1:88:A:SER:H	19	0.11
(1,572)	1:87:A:LEU:HD12	1:88:A:SER:H	19	0.11
(1,572)	1:87:A:LEU:HD13	1:88:A:SER:H	19	0.11
(1,572)	1:87:A:LEU:HD21	1:88:A:SER:H	19	0.11
(1,572)	1:87:A:LEU:HD22	1:88:A:SER:H	19	0.11
(1,572)	1:87:A:LEU:HD23	1:88:A:SER:H	19	0.11
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD21	11	0.11
(1,563)	1:60:A:ILE:HG21	1:87:A:LEU:HD12	12	0.11
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG2	12	0.11
(1,524)	1:84:A:VAL:HA	1:12:A:LYS:HG3	12	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	8	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	8	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	8	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	8	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	8	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	8	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	8	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	8	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	8	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	8	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	8	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	8	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	20	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	20	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	20	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	20	0.11
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	20	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	20	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	20	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	20	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	20	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	20	0.11
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	20	0.11
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD1	4	0.11
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD2	4	0.11
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD1	4	0.11
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD2	4	0.11
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD1	4	0.11
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD2	4	0.11
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD1	4	0.11
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD2	4	0.11
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD1	4	0.11
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD2	4	0.11
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD1	4	0.11
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD2	4	0.11
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD1	8	0.11
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD2	8	0.11
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD1	8	0.11
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD2	8	0.11
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD1	8	0.11
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD2	8	0.11
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD1	8	0.11
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD2	8	0.11
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD1	8	0.11
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD2	8	0.11
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD1	8	0.11
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD2	8	0.11
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB2	19	0.11
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB3	19	0.11
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	14	0.11
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	14	0.11
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB2	16	0.11
(1,474)	1:79:A:ILE:HA	1:78:A:LYS:HB3	16	0.11
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	6	0.11
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	14	0.11
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	14	0.11
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	3	0.11
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	3	0.11
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	17	0.11
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	17	0.11
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	19	0.11
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	19	0.11
(1,435)	1:37:A:VAL:HG11	1:75:A:VAL:HB	17	0.11
(1,435)	1:37:A:VAL:HG12	1:75:A:VAL:HB	17	0.11
(1,435)	1:37:A:VAL:HG13	1:75:A:VAL:HB	17	0.11
(1,435)	1:37:A:VAL:HG21	1:75:A:VAL:HB	17	0.11
(1,435)	1:37:A:VAL:HG22	1:75:A:VAL:HB	17	0.11
(1,435)	1:37:A:VAL:HG23	1:75:A:VAL:HB	17	0.11
(1,421)	1:71:A:GLN:HB2	1:73:A:THR:HG22	19	0.11
(1,409)	1:69:A:THR:HG1	1:54:A:LEU:HA	5	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	1	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	1	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	8	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	8	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	12	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	12	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	19	0.11
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	19	0.11
(1,405)	1:40:A:LEU:HG	1:68:A:LEU:H	11	0.11
(1,379)	1:42:A:PRO:HA	1:66:A:ILE:HG13	16	0.11
(1,341)	1:64:A:ASP:HB3	1:43:A:ILE:HG13	5	0.11
(1,326)	1:60:A:ILE:HG21	1:58:A:ILE:HG12	10	0.11
(1,326)	1:60:A:ILE:HG21	1:58:A:ILE:HG12	13	0.11
(1,320)	1:58:A:ILE:HB	1:58:A:ILE:H	7	0.11
(1,320)	1:58:A:ILE:HB	1:58:A:ILE:H	10	0.11
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	8	0.11
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	8	0.11
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	8	0.11
(1,314)	1:58:A:ILE:HD11	1:58:A:ILE:HA	14	0.11
(1,314)	1:58:A:ILE:HD12	1:58:A:ILE:HA	14	0.11
(1,314)	1:58:A:ILE:HD13	1:58:A:ILE:HA	14	0.11
(1,312)	1:58:A:ILE:HG13	1:57:A:THR:HB	9	0.11
(1,311)	1:58:A:ILE:HG13	1:57:A:THR:HB	9	0.11
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	12	0.11
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	16	0.11
(1,282)	1:47:A:ASP:HB2	1:48:A:LYS:HA	5	0.11
(1,282)	1:47:A:ASP:HB3	1:48:A:LYS:HA	5	0.11
(1,278)	1:48:A:LYS:HD3	1:43:A:ILE:HG21	6	0.11
(1,278)	1:48:A:LYS:HD2	1:43:A:ILE:HG21	17	0.11
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	2	0.11
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	4	0.11
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	8	0.11
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	9	0.11
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	11	0.11
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	12	0.11
(1,262)	1:43:A:ILE:HD11	1:43:A:ILE:HB	4	0.11
(1,262)	1:43:A:ILE:HD12	1:43:A:ILE:HB	4	0.11
(1,262)	1:43:A:ILE:HD13	1:43:A:ILE:HB	4	0.11
(1,262)	1:43:A:ILE:HD11	1:43:A:ILE:HB	11	0.11
(1,262)	1:43:A:ILE:HD12	1:43:A:ILE:HB	11	0.11
(1,262)	1:43:A:ILE:HD13	1:43:A:ILE:HB	11	0.11
(1,262)	1:43:A:ILE:HD11	1:43:A:ILE:HB	12	0.11
(1,262)	1:43:A:ILE:HD12	1:43:A:ILE:HB	12	0.11
(1,262)	1:43:A:ILE:HD13	1:43:A:ILE:HB	12	0.11
(1,261)	1:43:A:ILE:HG13	1:42:A:PRO:HA	7	0.11
(1,251)	1:19:A:PRO:HG2	1:41:A:THR:HB	9	0.11
(1,251)	1:19:A:PRO:HG3	1:41:A:THR:HB	9	0.11
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	13	0.11
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	13	0.11
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	15	0.11
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	15	0.11
(1,239)	1:39:A:PRO:HB2	1:40:A:LEU:HA	16	0.11
(1,239)	1:39:A:PRO:HB3	1:40:A:LEU:HA	16	0.11
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB2	3	0.11
(1,238)	1:40:A:LEU:HG	1:20:A:TYR:HB3	3	0.11
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	3	0.11
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	3	0.11
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	3	0.11
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	3	0.11
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	3	0.11
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	3	0.11
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	3	0.11
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	3	0.11
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	3	0.11
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	3	0.11
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	3	0.11
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	5	0.11
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	5	0.11
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	5	0.11
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	5	0.11
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	5	0.11
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	5	0.11
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	5	0.11
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	5	0.11
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	5	0.11
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	5	0.11
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	5	0.11
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	5	0.11
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB2	12	0.11
(1,192)	1:36:A:LEU:HB2	1:25:A:GLN:HB3	12	0.11
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB2	12	0.11
(1,192)	1:36:A:LEU:HB3	1:25:A:GLN:HB3	12	0.11
(1,186)	1:34:A:THR:HA	1:34:A:THR:HG22	1	0.11
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB2	18	0.11
(1,169)	1:26:A:SER:HA	1:29:A:LEU:HB3	18	0.11
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	9	0.11
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	10	0.11
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	16	0.11
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	17	0.11
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	19	0.11
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG11	10	0.11
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG12	10	0.11
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG13	10	0.11
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG21	10	0.11
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG22	10	0.11
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG23	10	0.11
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	11	0.11
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	11	0.11
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	18	0.11
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	18	0.11
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	19	0.11
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	19	0.11
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	11	0.11
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	11	0.11
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	1	0.11
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	1	0.11
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	5	0.11
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	11	0.11
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	11	0.11
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	14	0.11
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	14	0.11
(1,3141)	1:26:B:SER:H	1:25:B:GLN:HA	4	0.1
(1,3141)	1:26:B:SER:H	1:25:B:GLN:HA	14	0.1
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	10	0.1
(1,3097)	1:5:B:THR:H	1:5:B:THR:HB	12	0.1
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB2	19	0.1
(1,3090)	1:100:B:PHE:H	1:101:B:LEU:HB3	19	0.1
(1,3086)	1:88:B:SER:H	1:90:B:PHE:H	5	0.1
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	6	0.1
(1,3080)	1:86:B:GLU:H	1:87:B:LEU:HA	20	0.1
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB2	12	0.1
(1,3072)	1:71:B:GLN:H	1:72:B:MET:HB3	12	0.1
(1,3069)	1:66:B:ILE:H	1:43:B:ILE:HG13	4	0.1
(1,3063)	1:60:B:ILE:H	1:59:B:HIS:H	15	0.1
(1,3060)	1:58:B:ILE:H	1:57:B:THR:HB	2	0.1
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	7	0.1
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	7	0.1
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB2	20	0.1
(1,3051)	1:26:B:SER:H	1:36:B:LEU:HB3	20	0.1
(1,3049)	1:32:B:LEU:H	1:34:B:THR:H	20	0.1
(1,2945)	1:71:A:GLN:H	1:68:A:LEU:HB2	19	0.1
(1,2945)	1:71:A:GLN:H	1:68:A:LEU:HB3	19	0.1
(1,2839)	1:5:A:THR:H	1:5:A:THR:HB	8	0.1
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	5	0.1
(1,2822)	1:86:A:GLU:H	1:87:A:LEU:HA	17	0.1
(1,2805)	1:60:A:ILE:H	1:59:A:HIS:H	8	0.1
(1,2803)	1:60:A:ILE:H	1:58:A:ILE:HG21	8	0.1
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	3	0.1
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	17	0.1
(1,2802)	1:58:A:ILE:H	1:57:A:THR:HB	20	0.1
(1,2794)	1:36:A:LEU:H	1:26:A:SER:H	3	0.1
(1,2791)	1:32:A:LEU:H	1:34:A:THR:H	19	0.1
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB2	6	0.1
(1,2788)	1:32:A:LEU:H	1:2:A:SER:HB3	6	0.1
(1,2760)	1:103:B:THR:HG21	1:103:B:THR:HA	1	0.1
(1,2760)	1:103:B:THR:HG21	1:103:B:THR:HA	14	0.1
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	1	0.1
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	1	0.1
(1,2541)	1:79:B:ILE:HD11	1:75:B:VAL:HB	3	0.1
(1,2541)	1:79:B:ILE:HD12	1:75:B:VAL:HB	3	0.1
(1,2541)	1:79:B:ILE:HD13	1:75:B:VAL:HB	3	0.1
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB2	6	0.1
(1,2343)	1:42:B:PRO:HB2	1:44:B:GLU:HB3	6	0.1
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB2	6	0.1
(1,2343)	1:42:B:PRO:HB3	1:44:B:GLU:HB3	6	0.1
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB2	13	0.1
(1,2276)	1:25:B:GLN:HB2	1:36:B:LEU:HB3	13	0.1
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB2	13	0.1
(1,2276)	1:25:B:GLN:HB3	1:36:B:LEU:HB3	13	0.1
(1,2121)	1:105:B:ILE:HG13	1:99:B:ASP:HA	6	0.1
(1,2116)	1:103:B:THR:HB	1:102:B:ILE:HG13	13	0.1
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD11	16	0.1
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD12	16	0.1
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD13	16	0.1
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD21	16	0.1
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD22	16	0.1
(1,2109)	1:102:B:ILE:HA	1:101:B:LEU:HD23	16	0.1
(1,2092)	1:101:B:LEU:HD11	1:72:B:MET:HB2	7	0.1
(1,2092)	1:101:B:LEU:HD11	1:72:B:MET:HB3	7	0.1
(1,2092)	1:101:B:LEU:HD12	1:72:B:MET:HB2	7	0.1
(1,2092)	1:101:B:LEU:HD12	1:72:B:MET:HB3	7	0.1
(1,2092)	1:101:B:LEU:HD13	1:72:B:MET:HB2	7	0.1
(1,2092)	1:101:B:LEU:HD13	1:72:B:MET:HB3	7	0.1
(1,2092)	1:101:B:LEU:HD21	1:72:B:MET:HB2	7	0.1
(1,2092)	1:101:B:LEU:HD21	1:72:B:MET:HB3	7	0.1
(1,2092)	1:101:B:LEU:HD22	1:72:B:MET:HB2	7	0.1
(1,2092)	1:101:B:LEU:HD22	1:72:B:MET:HB3	7	0.1
(1,2092)	1:101:B:LEU:HD23	1:72:B:MET:HB2	7	0.1
(1,2092)	1:101:B:LEU:HD23	1:72:B:MET:HB3	7	0.1
(1,2062)	1:96:B:ALA:HA	1:99:B:ASP:HA	19	0.1
(1,2034)	1:91:B:ARG:HB2	1:95:B:ILE:HG13	2	0.1
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	2	0.1
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	11	0.1
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	14	0.1
(1,2025)	1:94:B:ILE:HG13	1:22:B:VAL:HB	15	0.1
(1,2023)	1:94:B:ILE:HG13	1:4:B:PHE:HE1	1	0.1
(1,1989)	1:88:B:SER:HB2	1:91:B:ARG:H	14	0.1
(1,1989)	1:88:B:SER:HB3	1:91:B:ARG:H	14	0.1
(1,1969)	1:58:B:ILE:HB	1:90:B:PHE:HZ	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1956)	1:87:B:LEU:HD11	1:88:B:SER:H	2	0.1
(1,1956)	1:87:B:LEU:HD12	1:88:B:SER:H	2	0.1
(1,1956)	1:87:B:LEU:HD13	1:88:B:SER:H	2	0.1
(1,1956)	1:87:B:LEU:HD21	1:88:B:SER:H	2	0.1
(1,1956)	1:87:B:LEU:HD22	1:88:B:SER:H	2	0.1
(1,1956)	1:87:B:LEU:HD23	1:88:B:SER:H	2	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	9	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	9	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	9	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	9	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	9	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	9	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	9	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	9	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	9	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	9	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	9	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	9	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG11	17	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG12	17	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG13	17	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG21	17	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG22	17	0.1
(1,1906)	1:7:B:TYR:HB2	1:84:B:VAL:HG23	17	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG11	17	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG12	17	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG13	17	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG21	17	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG22	17	0.1
(1,1906)	1:7:B:TYR:HB3	1:84:B:VAL:HG23	17	0.1
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD1	9	0.1
(1,1872)	1:80:B:LEU:HD11	1:21:B:PHE:HD2	9	0.1
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD1	9	0.1
(1,1872)	1:80:B:LEU:HD12	1:21:B:PHE:HD2	9	0.1
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD1	9	0.1
(1,1872)	1:80:B:LEU:HD13	1:21:B:PHE:HD2	9	0.1
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD1	9	0.1
(1,1872)	1:80:B:LEU:HD21	1:21:B:PHE:HD2	9	0.1
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD1	9	0.1
(1,1872)	1:80:B:LEU:HD22	1:21:B:PHE:HD2	9	0.1
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD1	9	0.1
(1,1872)	1:80:B:LEU:HD23	1:21:B:PHE:HD2	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	14	0.1
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	14	0.1
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	14	0.1
(1,1862)	1:79:B:ILE:HD11	1:79:B:ILE:HA	15	0.1
(1,1862)	1:79:B:ILE:HD12	1:79:B:ILE:HA	15	0.1
(1,1862)	1:79:B:ILE:HD13	1:79:B:ILE:HA	15	0.1
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG11	13	0.1
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG12	13	0.1
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG13	13	0.1
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG21	13	0.1
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG22	13	0.1
(1,1856)	1:79:B:ILE:HD11	1:75:B:VAL:HG23	13	0.1
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG11	13	0.1
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG12	13	0.1
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG13	13	0.1
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG21	13	0.1
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG22	13	0.1
(1,1856)	1:79:B:ILE:HD12	1:75:B:VAL:HG23	13	0.1
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG11	13	0.1
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG12	13	0.1
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG13	13	0.1
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG21	13	0.1
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG22	13	0.1
(1,1856)	1:79:B:ILE:HD13	1:75:B:VAL:HG23	13	0.1
(1,1854)	1:79:B:ILE:HD11	1:21:B:PHE:HD1	13	0.1
(1,1854)	1:79:B:ILE:HD11	1:21:B:PHE:HD2	13	0.1
(1,1854)	1:79:B:ILE:HD12	1:21:B:PHE:HD1	13	0.1
(1,1854)	1:79:B:ILE:HD12	1:21:B:PHE:HD2	13	0.1
(1,1854)	1:79:B:ILE:HD13	1:21:B:PHE:HD1	13	0.1
(1,1854)	1:79:B:ILE:HD13	1:21:B:PHE:HD2	13	0.1
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	10	0.1
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	10	0.1
(1,1849)	1:78:B:LYS:HD2	1:78:B:LYS:HA	15	0.1
(1,1849)	1:78:B:LYS:HD3	1:78:B:LYS:HA	15	0.1
(1,1819)	1:37:B:VAL:HG11	1:75:B:VAL:HB	18	0.1
(1,1819)	1:37:B:VAL:HG12	1:75:B:VAL:HB	18	0.1
(1,1819)	1:37:B:VAL:HG13	1:75:B:VAL:HB	18	0.1
(1,1819)	1:37:B:VAL:HG21	1:75:B:VAL:HB	18	0.1
(1,1819)	1:37:B:VAL:HG22	1:75:B:VAL:HB	18	0.1
(1,1819)	1:37:B:VAL:HG23	1:75:B:VAL:HB	18	0.1
(1,1809)	1:74:B:SER:HB2	1:35:B:ARG:HA	4	0.1
(1,1809)	1:74:B:SER:HB3	1:35:B:ARG:HA	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1776)	1:67:B:MET:HG2	1:21:B:PHE:HA	2	0.1
(1,1776)	1:67:B:MET:HG3	1:21:B:PHE:HA	2	0.1
(1,1698)	1:58:B:ILE:HD11	1:58:B:ILE:HA	4	0.1
(1,1698)	1:58:B:ILE:HD12	1:58:B:ILE:HA	4	0.1
(1,1698)	1:58:B:ILE:HD13	1:58:B:ILE:HA	4	0.1
(1,1691)	1:57:B:THR:HA	1:58:B:ILE:HA	13	0.1
(1,1690)	1:56:B:PRO:HB2	1:58:B:ILE:HG13	16	0.1
(1,1662)	1:48:B:LYS:HD2	1:43:B:ILE:HG21	8	0.1
(1,1646)	1:43:B:ILE:HD11	1:43:B:ILE:HB	2	0.1
(1,1646)	1:43:B:ILE:HD12	1:43:B:ILE:HB	2	0.1
(1,1646)	1:43:B:ILE:HD13	1:43:B:ILE:HB	2	0.1
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	2	0.1
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	2	0.1
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB2	5	0.1
(1,1632)	1:40:B:LEU:HG	1:40:B:LEU:HB3	5	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	4	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	4	0.1
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	4	0.1
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	4	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	4	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	4	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	4	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	4	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	4	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	4	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	4	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	4	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	9	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	9	0.1
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	9	0.1
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	9	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	9	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	9	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	9	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	9	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	9	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	9	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	9	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	9	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	10	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	10	0.1
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	10	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	10	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	10	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	10	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	10	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	10	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	10	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	10	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	10	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB2	17	0.1
(1,1617)	1:37:B:VAL:HG11	1:39:B:PRO:HB3	17	0.1
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB2	17	0.1
(1,1617)	1:37:B:VAL:HG12	1:39:B:PRO:HB3	17	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB2	17	0.1
(1,1617)	1:37:B:VAL:HG13	1:39:B:PRO:HB3	17	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB2	17	0.1
(1,1617)	1:37:B:VAL:HG21	1:39:B:PRO:HB3	17	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB2	17	0.1
(1,1617)	1:37:B:VAL:HG22	1:39:B:PRO:HB3	17	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB2	17	0.1
(1,1617)	1:37:B:VAL:HG23	1:39:B:PRO:HB3	17	0.1
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB2	13	0.1
(1,1576)	1:36:B:LEU:HB2	1:25:B:GLN:HB3	13	0.1
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB2	13	0.1
(1,1576)	1:36:B:LEU:HB3	1:25:B:GLN:HB3	13	0.1
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	6	0.1
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	9	0.1
(1,1535)	1:24:B:VAL:HA	1:25:B:GLN:HA	15	0.1
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG11	18	0.1
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG12	18	0.1
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG13	18	0.1
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG21	18	0.1
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG22	18	0.1
(1,1526)	1:22:B:VAL:HA	1:24:B:VAL:HG23	18	0.1
(1,1501)	1:22:B:VAL:HG11	1:21:B:PHE:HD1	19	0.1
(1,1501)	1:22:B:VAL:HG11	1:21:B:PHE:HD2	19	0.1
(1,1501)	1:22:B:VAL:HG12	1:21:B:PHE:HD1	19	0.1
(1,1501)	1:22:B:VAL:HG12	1:21:B:PHE:HD2	19	0.1
(1,1501)	1:22:B:VAL:HG13	1:21:B:PHE:HD1	19	0.1
(1,1501)	1:22:B:VAL:HG13	1:21:B:PHE:HD2	19	0.1
(1,1501)	1:22:B:VAL:HG21	1:21:B:PHE:HD1	19	0.1
(1,1501)	1:22:B:VAL:HG21	1:21:B:PHE:HD2	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:22:B:VAL:HG22	1:21:B:PHE:HD1	19	0.1
(1,1501)	1:22:B:VAL:HG22	1:21:B:PHE:HD2	19	0.1
(1,1501)	1:22:B:VAL:HG23	1:21:B:PHE:HD1	19	0.1
(1,1501)	1:22:B:VAL:HG23	1:21:B:PHE:HD2	19	0.1
(1,1495)	1:6:B:LEU:HA	1:22:B:VAL:HA	6	0.1
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	10	0.1
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	10	0.1
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	12	0.1
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	12	0.1
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD1	18	0.1
(1,1481)	1:9:B:ASN:HA	1:21:B:PHE:HD2	18	0.1
(1,1440)	1:9:B:ASN:HB2	1:15:B:ALA:HA	3	0.1
(1,1440)	1:9:B:ASN:HB3	1:15:B:ALA:HA	3	0.1
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD2	18	0.1
(1,1432)	1:11:B:ASP:HA	1:10:B:LYS:HD3	18	0.1
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG2	18	0.1
(1,1425)	1:9:B:ASN:HA	1:8:B:LYS:HG3	18	0.1
(1,1412)	1:7:B:TYR:HB2	1:5:B:THR:HB	9	0.1
(1,1412)	1:7:B:TYR:HB3	1:5:B:THR:HB	9	0.1
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD11	3	0.1
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD12	3	0.1
(1,1236)	1:87:A:LEU:HD11	1:58:A:ILE:HD13	3	0.1
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD11	3	0.1
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD12	3	0.1
(1,1236)	1:87:A:LEU:HD12	1:58:A:ILE:HD13	3	0.1
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD11	3	0.1
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD12	3	0.1
(1,1236)	1:87:A:LEU:HD13	1:58:A:ILE:HD13	3	0.1
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD11	3	0.1
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD12	3	0.1
(1,1236)	1:87:A:LEU:HD21	1:58:A:ILE:HD13	3	0.1
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD11	3	0.1
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD12	3	0.1
(1,1236)	1:87:A:LEU:HD22	1:58:A:ILE:HD13	3	0.1
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD11	3	0.1
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD12	3	0.1
(1,1236)	1:87:A:LEU:HD23	1:58:A:ILE:HD13	3	0.1
(1,1157)	1:79:A:ILE:HD11	1:75:A:VAL:HB	7	0.1
(1,1157)	1:79:A:ILE:HD12	1:75:A:VAL:HB	7	0.1
(1,1157)	1:79:A:ILE:HD13	1:75:A:VAL:HB	7	0.1
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	12	0.1
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	12	0.1
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	12	0.1
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	12	0.1
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	12	0.1
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	13	0.1
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	13	0.1
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	13	0.1
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	13	0.1
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	13	0.1
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	13	0.1
(1,891)	1:24:A:VAL:HG11	1:36:A:LEU:HG	16	0.1
(1,891)	1:24:A:VAL:HG12	1:36:A:LEU:HG	16	0.1
(1,891)	1:24:A:VAL:HG13	1:36:A:LEU:HG	16	0.1
(1,891)	1:24:A:VAL:HG21	1:36:A:LEU:HG	16	0.1
(1,891)	1:24:A:VAL:HG22	1:36:A:LEU:HG	16	0.1
(1,891)	1:24:A:VAL:HG23	1:36:A:LEU:HG	16	0.1
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	1	0.1
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	3	0.1
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	13	0.1
(1,678)	1:96:A:ALA:HA	1:99:A:ASP:HA	18	0.1
(1,668)	1:98:A:ILE:HD11	1:24:A:VAL:HA	11	0.1
(1,668)	1:98:A:ILE:HD12	1:24:A:VAL:HA	11	0.1
(1,668)	1:98:A:ILE:HD13	1:24:A:VAL:HA	11	0.1
(1,641)	1:94:A:ILE:HG13	1:22:A:VAL:HB	20	0.1
(1,626)	1:91:A:ARG:HG2	1:92:A:ASN:HA	17	0.1
(1,626)	1:91:A:ARG:HG3	1:92:A:ASN:HA	17	0.1
(1,605)	1:88:A:SER:HB2	1:91:A:ARG:H	6	0.1
(1,605)	1:88:A:SER:HB3	1:91:A:ARG:H	6	0.1
(1,594)	1:89:A:THR:HG21	1:90:A:PHE:HB2	14	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	3	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	3	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	3	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	3	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	3	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	3	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	3	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	3	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	3	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	3	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	3	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	3	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	4	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	4	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	4	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	4	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	4	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	4	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	4	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	4	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	4	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	4	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	4	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG11	13	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG12	13	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG13	13	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG21	13	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG22	13	0.1
(1,522)	1:7:A:TYR:HB2	1:84:A:VAL:HG23	13	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG11	13	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG12	13	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG13	13	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG21	13	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG22	13	0.1
(1,522)	1:7:A:TYR:HB3	1:84:A:VAL:HG23	13	0.1
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD1	6	0.1
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD2	6	0.1
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD1	6	0.1
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD2	6	0.1
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD1	6	0.1
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD2	6	0.1
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD1	6	0.1
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD2	6	0.1
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD1	6	0.1
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD2	6	0.1
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD1	6	0.1
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD2	6	0.1
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD1	10	0.1
(1,488)	1:80:A:LEU:HD11	1:21:A:PHE:HD2	10	0.1
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD1	10	0.1
(1,488)	1:80:A:LEU:HD12	1:21:A:PHE:HD2	10	0.1
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD1	10	0.1
(1,488)	1:80:A:LEU:HD13	1:21:A:PHE:HD2	10	0.1
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD1	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:80:A:LEU:HD21	1:21:A:PHE:HD2	10	0.1
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD1	10	0.1
(1,488)	1:80:A:LEU:HD22	1:21:A:PHE:HD2	10	0.1
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD1	10	0.1
(1,488)	1:80:A:LEU:HD23	1:21:A:PHE:HD2	10	0.1
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB2	7	0.1
(1,484)	1:80:A:LEU:HA	1:7:A:TYR:HB3	7	0.1
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB2	1	0.1
(1,483)	1:80:A:LEU:HA	1:7:A:TYR:HB3	1	0.1
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG2	16	0.1
(1,467)	1:78:A:LYS:HA	1:78:A:LYS:HG3	16	0.1
(1,465)	1:78:A:LYS:HD2	1:78:A:LYS:HA	15	0.1
(1,465)	1:78:A:LYS:HD3	1:78:A:LYS:HA	15	0.1
(1,452)	1:77:A:VAL:HB	1:34:A:THR:HA	9	0.1
(1,420)	1:73:A:THR:HG1	1:39:A:PRO:HG3	5	0.1
(1,420)	1:73:A:THR:HG22	1:39:A:PRO:HG3	8	0.1
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	10	0.1
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	10	0.1
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	14	0.1
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	14	0.1
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB2	17	0.1
(1,406)	1:41:A:THR:HB	1:68:A:LEU:HB3	17	0.1
(1,405)	1:40:A:LEU:HG	1:68:A:LEU:H	9	0.1
(1,343)	1:58:A:ILE:HB	1:64:A:ASP:HA	1	0.1
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	11	0.1
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	19	0.1
(1,307)	1:57:A:THR:HA	1:58:A:ILE:HA	20	0.1
(1,278)	1:48:A:LYS:HD2	1:43:A:ILE:HG21	19	0.1
(1,263)	1:43:A:ILE:HB	1:43:A:ILE:HG13	5	0.1
(1,262)	1:43:A:ILE:HD11	1:43:A:ILE:HB	2	0.1
(1,262)	1:43:A:ILE:HD12	1:43:A:ILE:HB	2	0.1
(1,262)	1:43:A:ILE:HD13	1:43:A:ILE:HB	2	0.1
(1,251)	1:19:A:PRO:HG2	1:41:A:THR:HB	13	0.1
(1,251)	1:19:A:PRO:HG3	1:41:A:THR:HB	13	0.1
(1,251)	1:19:A:PRO:HG2	1:41:A:THR:HB	15	0.1
(1,251)	1:19:A:PRO:HG3	1:41:A:THR:HB	15	0.1
(1,248)	1:40:A:LEU:HG	1:40:A:LEU:HB2	7	0.1
(1,248)	1:40:A:LEU:HG	1:40:A:LEU:HB3	7	0.1
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB2	1	0.1
(1,233)	1:37:A:VAL:HG11	1:39:A:PRO:HB3	1	0.1
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB2	1	0.1
(1,233)	1:37:A:VAL:HG12	1:39:A:PRO:HB3	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB2	1	0.1
(1,233)	1:37:A:VAL:HG13	1:39:A:PRO:HB3	1	0.1
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB2	1	0.1
(1,233)	1:37:A:VAL:HG21	1:39:A:PRO:HB3	1	0.1
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB2	1	0.1
(1,233)	1:37:A:VAL:HG22	1:39:A:PRO:HB3	1	0.1
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB2	1	0.1
(1,233)	1:37:A:VAL:HG23	1:39:A:PRO:HB3	1	0.1
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	7	0.1
(1,151)	1:24:A:VAL:HA	1:25:A:GLN:HA	8	0.1
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG11	14	0.1
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG12	14	0.1
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG13	14	0.1
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG21	14	0.1
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG22	14	0.1
(1,142)	1:22:A:VAL:HA	1:24:A:VAL:HG23	14	0.1
(1,117)	1:22:A:VAL:HG11	1:21:A:PHE:HD1	13	0.1
(1,117)	1:22:A:VAL:HG11	1:21:A:PHE:HD2	13	0.1
(1,117)	1:22:A:VAL:HG12	1:21:A:PHE:HD1	13	0.1
(1,117)	1:22:A:VAL:HG12	1:21:A:PHE:HD2	13	0.1
(1,117)	1:22:A:VAL:HG13	1:21:A:PHE:HD1	13	0.1
(1,117)	1:22:A:VAL:HG13	1:21:A:PHE:HD2	13	0.1
(1,117)	1:22:A:VAL:HG21	1:21:A:PHE:HD1	13	0.1
(1,117)	1:22:A:VAL:HG21	1:21:A:PHE:HD2	13	0.1
(1,117)	1:22:A:VAL:HG22	1:21:A:PHE:HD1	13	0.1
(1,117)	1:22:A:VAL:HG22	1:21:A:PHE:HD2	13	0.1
(1,117)	1:22:A:VAL:HG23	1:21:A:PHE:HD1	13	0.1
(1,117)	1:22:A:VAL:HG23	1:21:A:PHE:HD2	13	0.1
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD1	6	0.1
(1,97)	1:9:A:ASN:HA	1:21:A:PHE:HD2	6	0.1
(1,56)	1:9:A:ASN:HB2	1:15:A:ALA:HA	10	0.1
(1,56)	1:9:A:ASN:HB3	1:15:A:ALA:HA	10	0.1
(1,56)	1:9:A:ASN:HB2	1:15:A:ALA:HA	11	0.1
(1,56)	1:9:A:ASN:HB3	1:15:A:ALA:HA	11	0.1
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	9	0.1
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	9	0.1
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG2	19	0.1
(1,41)	1:9:A:ASN:HA	1:8:A:LYS:HG3	19	0.1
(1,28)	1:7:A:TYR:HB2	1:5:A:THR:HB	3	0.1
(1,28)	1:7:A:TYR:HB3	1:5:A:THR:HB	3	0.1

10 Dihedral-angle violation analysis

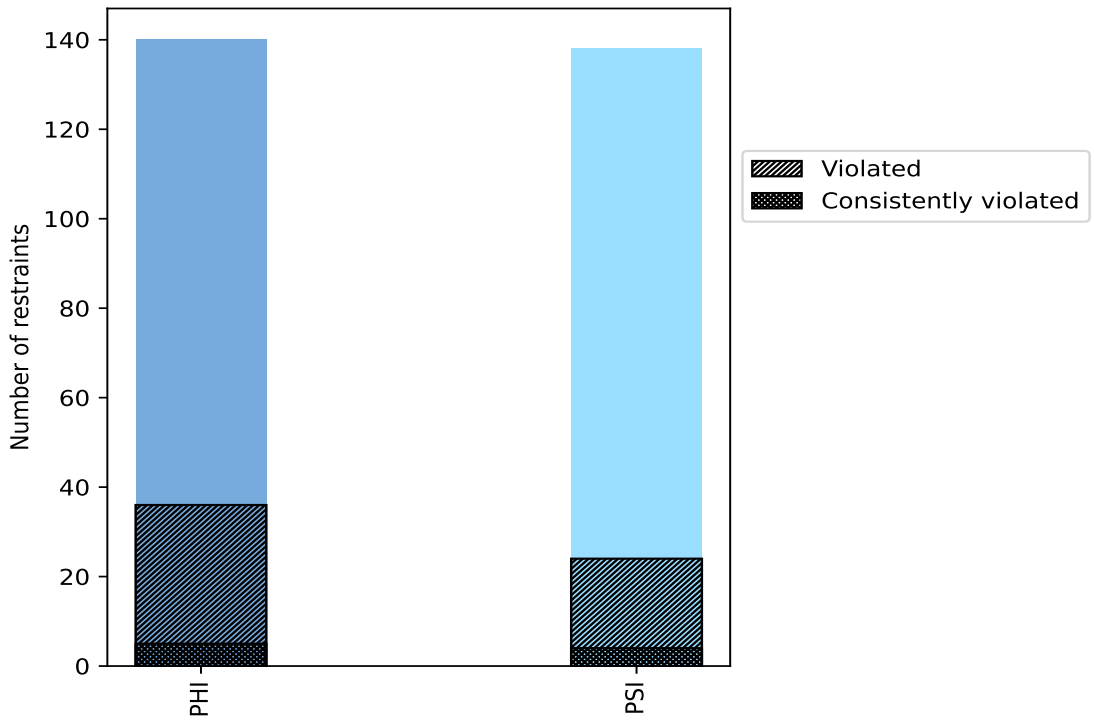
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	140	50.4	36	25.7	12.9	5	3.6	1.8
PSI	138	49.6	24	17.4	8.6	4	2.9	1.4
Total	278	100.0	60	21.6	21.6	9	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



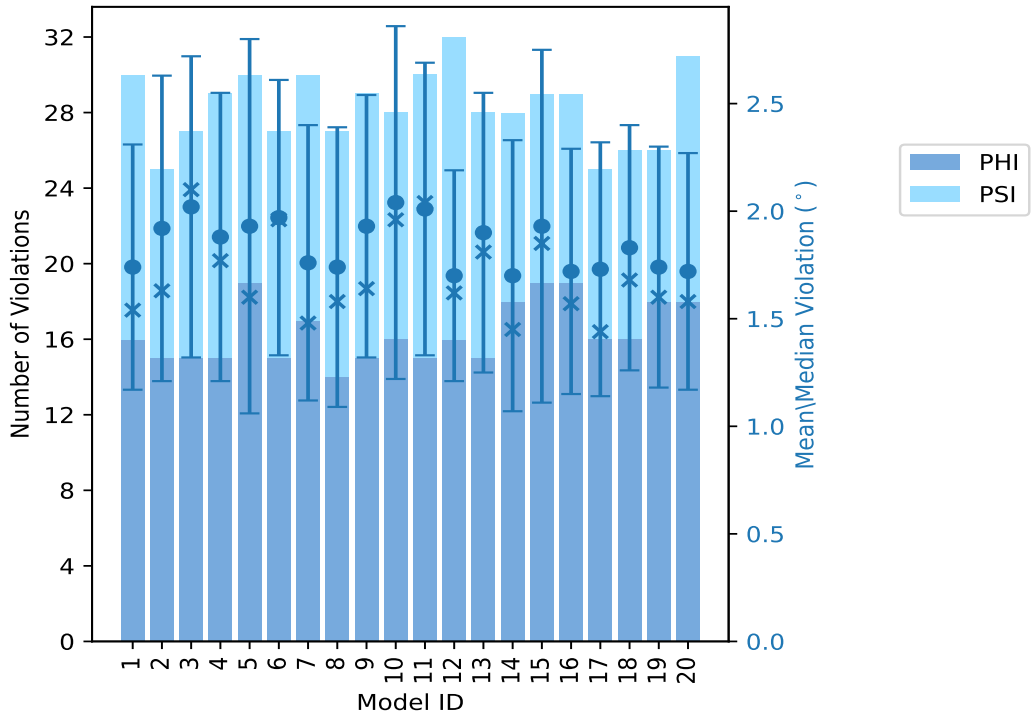
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	16	14	30	1.74	3.26	0.57	1.54
2	15	10	25	1.92	3.51	0.71	1.63
3	15	12	27	2.02	3.67	0.7	2.1
4	15	14	29	1.88	4.0	0.67	1.77
5	19	11	30	1.93	4.78	0.87	1.6
6	15	12	27	1.97	3.37	0.64	1.96
7	17	13	30	1.76	3.32	0.64	1.48
8	14	13	27	1.74	3.41	0.65	1.58
9	15	14	29	1.93	3.59	0.61	1.64
10	16	12	28	2.04	4.1	0.82	1.96
11	15	15	30	2.01	3.3	0.68	2.04
12	16	16	32	1.7	3.01	0.49	1.62
13	15	13	28	1.9	3.29	0.65	1.81
14	18	10	28	1.7	3.54	0.63	1.45
15	19	10	29	1.93	4.44	0.82	1.85
16	19	10	29	1.72	3.09	0.57	1.57
17	16	9	25	1.73	2.77	0.59	1.44
18	16	10	26	1.83	2.86	0.57	1.68
19	18	8	26	1.74	2.9	0.56	1.6
20	18	13	31	1.72	2.9	0.55	1.58

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	
PHI	PSI	Total	Count[1]	%
6	4	10	1	5.0
4	2	6	2	10.0
1	2	3	3	15.0
3	0	3	4	20.0
1	1	2	5	25.0
0	0	0	6	30.0
3	0	3	7	35.0
1	0	1	8	40.0
2	3	5	9	45.0
1	0	1	10	50.0
0	1	1	11	55.0

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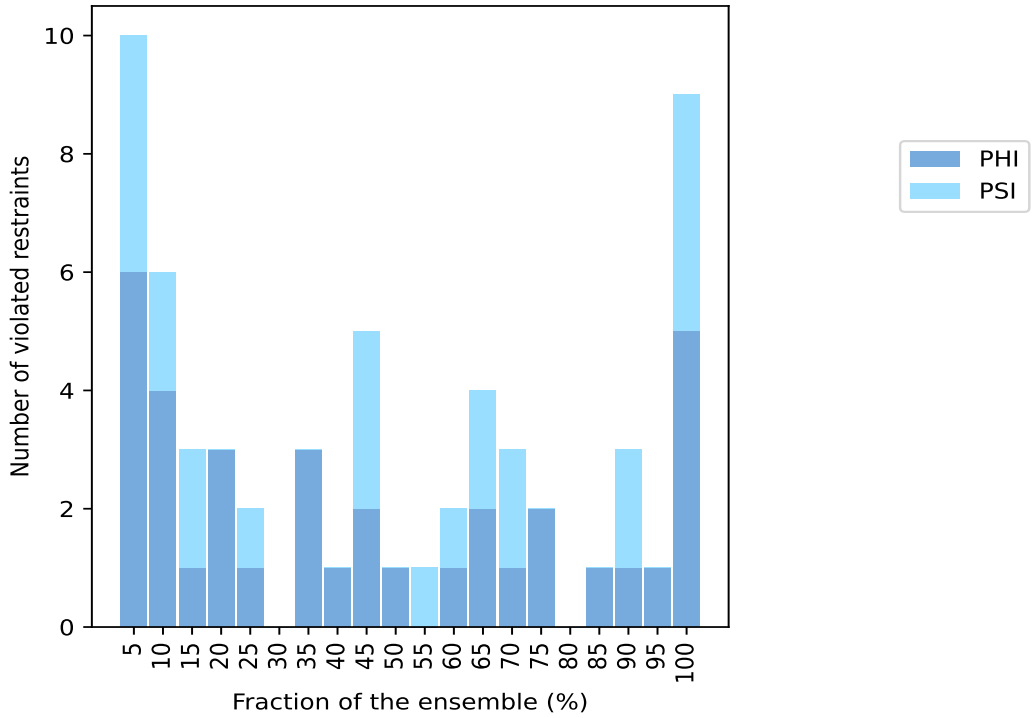
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	1	2	12	60.0
2	2	4	13	65.0
1	2	3	14	70.0
2	0	2	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
1	2	3	18	90.0
1	0	1	19	95.0
5	4	9	20	100.0

[1] Number of models with violations

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

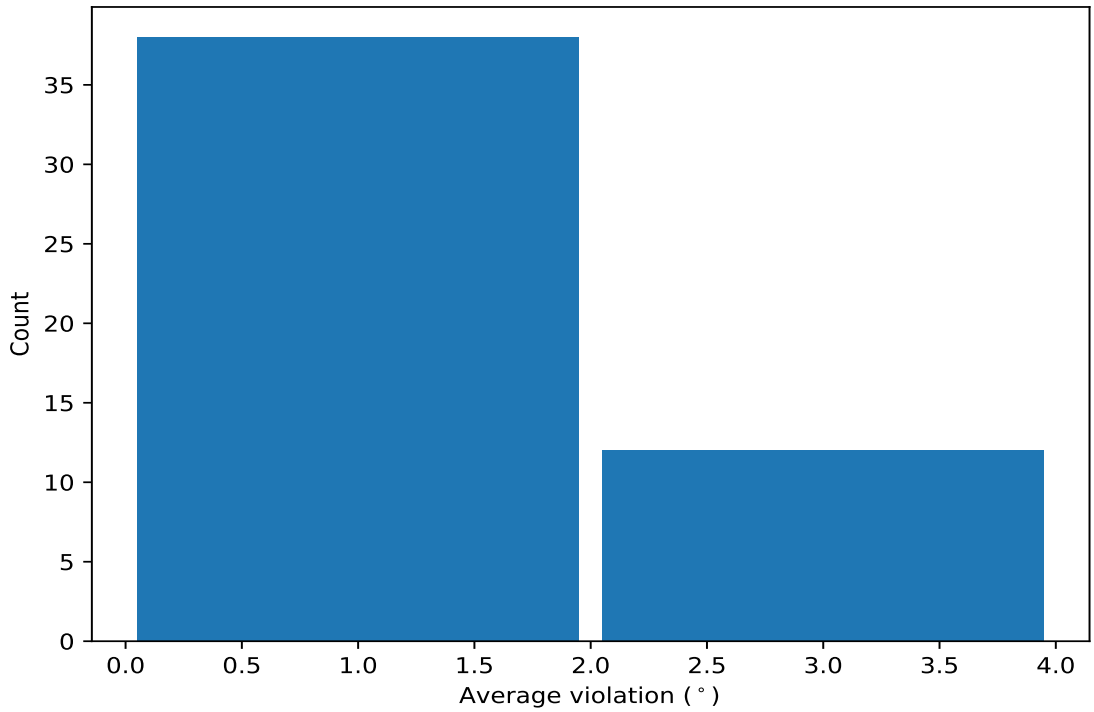


10.4 Most violated dihedral-angle restraints in the ensemble

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
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	20	2.47	0.45	2.44
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	20	2.4	0.46	2.3
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	20	2.37	0.34	2.34
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	20	2.35	0.59	2.22
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	20	2.3	0.4	2.34
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	20	2.27	0.36	2.3
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	20	2.24	0.76	2.17
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	20	1.92	0.74	1.61
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	20	1.57	0.4	1.46
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	19	1.81	0.32	1.9
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	18	2.14	0.61	2.11
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	18	1.89	0.73	1.68
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	18	1.8	0.4	1.83
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	17	2.06	0.59	1.96
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	15	1.4	0.34	1.31
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	15	1.39	0.16	1.45
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	14	2.15	0.88	1.96
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	14	1.75	0.5	1.67
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	14	1.3	0.19	1.33
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	13	2.85	0.88	3.1

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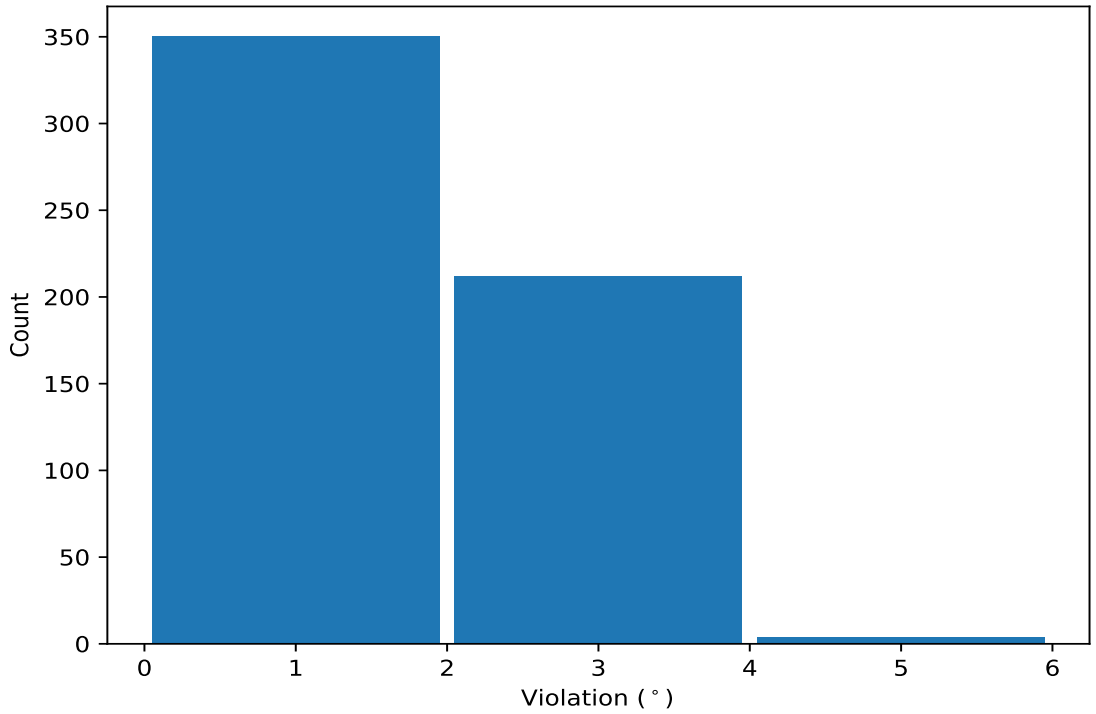
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	13	1.86	0.55	1.74
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	13	1.41	0.32	1.32
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	13	1.37	0.17	1.29
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	12	2.59	0.78	3.0
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	12	1.54	0.47	1.31
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	11	1.29	0.18	1.23
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	10	1.98	0.63	1.84
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	9	1.94	0.34	1.95
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	9	1.83	0.44	1.6
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	9	1.57	0.36	1.58
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	9	1.34	0.41	1.16
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	9	1.15	0.08	1.13
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	8	1.29	0.12	1.29
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	7	1.51	0.45	1.34
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	7	1.26	0.25	1.12
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	7	1.12	0.1	1.09
(1,210)	1:58:B:ILE:C	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	5	1.66	0.35	1.75
(1,165)	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:C	1:21:B:PHE:N	5	1.36	0.4	1.18
(1,17)	1:14:A:SER:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	4	1.24	0.08	1.23
(1,51)	1:37:A:VAL:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	4	1.12	0.15	1.04
(1,176)	1:27:B:ASP:C	1:28:B:LEU:N	1:28:B:LEU:CA	1:28:B:LEU:C	4	1.12	0.06	1.13
(1,11)	1:11:A:ASP:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	3	1.33	0.42	1.05
(1,86)	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	1:68:A:LEU:N	3	1.2	0.02	1.19
(1,225)	1:67:B:MET:N	1:67:B:MET:CA	1:67:B:MET:C	1:68:B:LEU:N	3	1.13	0.09	1.11
(1,185)	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	1:36:B:LEU:N	2	1.93	0.46	1.93
(1,5)	1:6:A:LEU:C	1:7:A:TYR:N	1:7:A:TYR:CA	1:7:A:TYR:C	2	1.28	0.03	1.28
(1,227)	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	1:69:B:THR:N	2	1.12	0.12	1.12
(1,47)	1:35:A:ARG:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	2	1.06	0.01	1.06
(1,156)	1:14:B:SER:C	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	2	1.06	0.01	1.06
(1,170)	1:22:B:VAL:C	1:23:B:ASP:N	1:23:B:ASP:CA	1:23:B:ASP:C	2	1.02	0.0	1.02

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	5	4.78
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	15	4.44
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	10	4.1
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	4	4.0
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	3	3.67
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	10	3.67
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	9	3.59
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	15	3.56
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	14	3.54
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	2	3.51
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	2	3.47
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	5	3.45
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	8	3.41
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	15	3.39
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	10	3.37
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	6	3.37
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	7	3.32
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	11	3.3
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	13	3.29
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	1	3.26
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	11	3.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	6	3.2
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	9	3.18
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	2	3.15
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	6	3.13
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	5	3.13
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	5	3.13
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	8	3.11
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	3	3.1
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	10	3.1
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	5	3.1
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	16	3.09
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	13	3.04
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	12	3.01
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	11	3.0
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	3	2.94
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	10	2.94
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	3	2.93
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	14	2.91
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	13	2.91
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	19	2.9
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	20	2.9
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	11	2.89
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	13	2.88
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	13	2.87
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	2	2.86
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	18	2.86
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	18	2.84
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	19	2.84
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	20	2.83
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	9	2.83
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	7	2.79
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	18	2.79
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	11	2.78
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	4	2.78
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	6	2.78
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	17	2.77
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	4	2.77
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	16	2.77
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	17	2.77
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	8	2.74
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	19	2.73
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	16	2.73
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	17	2.73
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	20	2.72
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	14	2.7
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	18	2.68
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	4	2.67
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	20	2.67
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	3	2.64
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	7	2.64
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	10	2.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	5	2.64
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	20	2.63
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	1	2.62
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	15	2.62
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	18	2.6
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	4	2.6
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	11	2.6
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	15	2.6
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	2	2.59
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	15	2.59
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	11	2.59
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	9	2.57
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	16	2.56
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	12	2.56
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	12	2.56
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	1	2.55
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	7	2.54
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	14	2.54
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	10	2.53
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	2	2.52
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	1	2.51
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	11	2.5
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	7	2.49
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	10	2.48
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	3	2.48
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	6	2.47
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	9	2.47
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	7	2.47
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	11	2.47
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	4	2.47
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	6	2.46
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	17	2.46
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	8	2.45
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	17	2.43
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	3	2.43
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	11	2.43
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	3	2.42
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	9	2.42
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	10	2.42
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	12	2.41
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	15	2.41
(1,185)	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	1:36:B:LEU:N	3	2.39
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	17	2.39
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	7	2.37
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	1	2.37
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	11	2.37
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	19	2.35
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	4	2.35
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	16	2.35
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	14	2.35
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	6	2.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	4	2.34
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	7	2.34
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	12	2.34
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	15	2.33
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	12	2.33
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	19	2.33
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	1	2.33
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	11	2.33
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	8	2.32
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	3	2.31
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	5	2.31
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	8	2.31
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	7	2.3
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	18	2.3
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	16	2.3
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	7	2.29
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	15	2.29
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	19	2.29
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	9	2.28
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	13	2.28
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	8	2.28
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	11	2.28
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	5	2.27
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	14	2.27
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	9	2.27
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	3	2.26
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	6	2.26
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	11	2.25
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	18	2.25
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	10	2.25
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	3	2.25
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	3	2.24
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	9	2.24
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	13	2.24
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	16	2.23
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	2	2.23
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	13	2.23
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	13	2.23
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	9	2.22
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	5	2.22
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	14	2.21
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	9	2.21
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	1	2.21
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	15	2.19
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	4	2.19
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	17	2.19
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	2	2.18
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	1	2.18
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	5	2.18
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	2	2.18
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	10	2.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	20	2.17
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	13	2.17
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	7	2.16
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	20	2.16
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	10	2.16
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	13	2.15
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	6	2.15
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	17	2.15
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	9	2.15
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	1	2.13
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	20	2.12
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	11	2.12
(1,165)	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:C	1:21:B:PHE:N	4	2.12
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	5	2.12
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	19	2.12
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	4	2.12
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	5	2.11
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	3	2.1
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	10	2.1
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	18	2.09
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	16	2.09
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	4	2.09
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	13	2.09
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	15	2.09
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	20	2.08
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	18	2.08
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	18	2.07
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	3	2.06
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	17	2.06
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	12	2.04
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	6	2.04
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	12	2.03
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	15	2.03
(1,210)	1:58:B:ILE:C	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1	2.02
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	10	2.02
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	6	2.01
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	17	2.01
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	19	2.01
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	15	2.0
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	8	2.0
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	20	2.0
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	6	2.0
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	9	1.98
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	18	1.97
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	11	1.97
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	14	1.97
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	8	1.97
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	6	1.96
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	6	1.96
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	1	1.96
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	1	1.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	6	1.95
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	12	1.95
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	8	1.95
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	11	1.93
(1,11)	1:11:A:ASP:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	19	1.93
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	19	1.92
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	6	1.92
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	19	1.92
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	7	1.92
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	7	1.91
(1,164)	1:19:B:PRO:C	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:C	15	1.91
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1	1.91
(1,210)	1:58:B:ILE:C	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	10	1.9
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	3	1.9
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	16	1.9
(1,52)	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	1:39:A:PRO:N	8	1.9
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	12	1.89
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	16	1.89
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	6	1.87
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	13	1.86
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	11	1.86
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	15	1.85
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	2	1.85
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1	1.84
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	13	1.84
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	4	1.84
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	16	1.83
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	9	1.82
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	4	1.81
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	16	1.81
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	18	1.81
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	14	1.8
(1,191)	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	1:39:B:PRO:N	12	1.79
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	5	1.79
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	14	1.78
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	2	1.78
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	14	1.78
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	20	1.78
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	13	1.77
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	4	1.77
(1,210)	1:58:B:ILE:C	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	2	1.75
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	20	1.75
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	11	1.75
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	6	1.75
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	10	1.74
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	5	1.73
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	10	1.73
(1,212)	1:59:B:HIS:C	1:60:B:ILE:N	1:60:B:ILE:CA	1:60:B:ILE:C	3	1.71
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	19	1.71
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	13	1.71
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	17	1.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	8	1.69
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	10	1.69
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	16	1.69
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	18	1.68
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	18	1.68
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	12	1.68
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	5	1.67
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	13	1.67
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	3	1.67
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	11	1.66
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	19	1.65
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	12	1.65
(1,210)	1:58:B:ILE:C	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	9	1.64
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	9	1.63
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	4	1.63
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	12	1.63
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	2	1.63
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	20	1.63
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	20	1.62
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	12	1.62
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	15	1.62
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	12	1.62
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	6	1.62
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	12	1.62
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	8	1.61
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	9	1.61
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	12	1.6
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	12	1.6
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	2	1.6
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	18	1.6
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	20	1.6
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	16	1.6
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	14	1.58
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	9	1.58
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	15	1.58
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	8	1.58
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	9	1.58
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	20	1.58
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	9	1.58
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	9	1.58
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	20	1.58
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	7	1.57
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	16	1.57
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	8	1.57
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	20	1.57
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	1	1.57
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	6	1.57
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	2	1.56
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	9	1.55
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	19	1.55
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	19	1.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	7	1.54
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	19	1.54
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	20	1.53
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	4	1.53
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	13	1.53
(1,160)	1:16:B:LYS:C	1:17:B:THR:N	1:17:B:THR:CA	1:17:B:THR:C	19	1.53
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	16	1.53
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	5	1.52
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	12	1.52
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	5	1.52
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	5	1.51
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	1	1.5
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	17	1.5
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	4	1.5
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	14	1.49
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	5	1.49
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	18	1.49
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	9	1.48
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	13	1.48
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	10	1.48
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	18	1.48
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	2	1.48
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	13	1.48
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	15	1.48
(1,185)	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	1:36:B:LEU:N	14	1.47
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	1	1.47
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	12	1.47
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	9	1.47
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	16	1.46
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	20	1.46
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	5	1.46
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	3	1.45
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	18	1.45
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	16	1.45
(1,21)	1:16:A:LYS:C	1:17:A:THR:N	1:17:A:THR:CA	1:17:A:THR:C	2	1.45
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	5	1.44
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	4	1.44
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	17	1.44
(1,102)	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	1:80:A:LEU:N	1	1.44
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	17	1.44
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	13	1.44
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	17	1.43
(1,132)	1:99:A:ASP:C	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	14	1.43
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	16	1.43
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	14	1.42
(1,241)	1:79:B:ILE:N	1:79:B:ILE:CA	1:79:B:ILE:C	1:80:B:LEU:N	2	1.42
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	4	1.42
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	4	1.42
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	7	1.42
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	16	1.41
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	1	1.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	4	1.41
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	14	1.41
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	9	1.4
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	7	1.4
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	1	1.4
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	7	1.39
(1,165)	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:C	1:21:B:PHE:N	11	1.39
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	18	1.38
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	6	1.37
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	12	1.37
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	12	1.37
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	15	1.37
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	18	1.37
(1,51)	1:37:A:VAL:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	2	1.37
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	3	1.36
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	15	1.36
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	5	1.35
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	6	1.35
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	19	1.35
(1,17)	1:14:A:SER:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	18	1.35
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	4	1.34
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	3	1.34
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	10	1.34
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	20	1.34
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	3	1.34
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	11	1.33
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	14	1.33
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	15	1.33
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	4	1.32
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	5	1.32
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	2	1.32
(1,271)	1:99:B:ASP:C	1:100:B:PHE:N	1:100:B:PHE:CA	1:100:B:PHE:C	19	1.31
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	10	1.31
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	8	1.31
(1,73)	1:59:A:HIS:C	1:60:A:ILE:N	1:60:A:ILE:CA	1:60:A:ILE:C	9	1.31
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	7	1.31
(1,5)	1:6:A:LEU:C	1:7:A:TYR:N	1:7:A:TYR:CA	1:7:A:TYR:C	14	1.31
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	11	1.3
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	12	1.3
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	15	1.3
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	2	1.29
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	10	1.29
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	17	1.29
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	8	1.29
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	20	1.28
(1,211)	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	1:60:B:ILE:N	17	1.28
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	8	1.28
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	8	1.27
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	14	1.27
(1,131)	1:99:A:ASP:N	1:99:A:ASP:CA	1:99:A:ASP:C	1:100:A:PHE:N	11	1.27
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	13	1.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	17	1.27
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	4	1.27
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	14	1.27
(1,17)	1:14:A:SER:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	2	1.27
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	18	1.26
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	16	1.26
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	14	1.26
(1,5)	1:6:A:LEU:C	1:7:A:TYR:N	1:7:A:TYR:CA	1:7:A:TYR:C	20	1.26
(1,225)	1:67:B:MET:N	1:67:B:MET:CA	1:67:B:MET:C	1:68:B:LEU:N	8	1.25
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	1	1.25
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	1	1.25
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	20	1.25
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	7	1.25
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	10	1.25
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	7	1.25
(1,31)	1:22:A:VAL:C	1:23:A:ASP:N	1:23:A:ASP:CA	1:23:A:ASP:C	20	1.25
(1,227)	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	1:69:B:THR:N	12	1.24
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	18	1.24
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	9	1.24
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	19	1.24
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	16	1.23
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	10	1.23
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	20	1.23
(1,86)	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	1:68:A:LEU:N	7	1.23
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	12	1.23
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	2	1.22
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	12	1.22
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	5	1.21
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	11	1.21
(1,72)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:ILE:N	2	1.21
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	11	1.21
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	20	1.2
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	1	1.2
(1,219)	1:64:B:ASP:N	1:64:B:ASP:CA	1:64:B:ASP:C	1:65:B:PHE:N	15	1.2
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	13	1.2
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	17	1.2
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	3	1.2
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	4	1.2
(1,86)	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	1:68:A:LEU:N	13	1.19
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	17	1.18
(1,221)	1:65:B:PHE:N	1:65:B:PHE:CA	1:65:B:PHE:C	1:66:B:ILE:N	12	1.18
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	5	1.18
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	19	1.18
(1,176)	1:27:B:ASP:C	1:28:B:LEU:N	1:28:B:LEU:CA	1:28:B:LEU:C	17	1.18
(1,165)	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:C	1:21:B:PHE:N	1	1.18
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	6	1.18
(1,71)	1:58:A:ILE:C	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	7	1.18
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	15	1.18
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	8	1.18
(1,17)	1:14:A:SER:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	16	1.18
(1,199)	1:44:B:GLU:N	1:44:B:GLU:CA	1:44:B:GLU:C	1:45:B:LEU:N	13	1.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	15	1.17
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	3	1.17
(1,86)	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	1:68:A:LEU:N	16	1.17
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	2	1.17
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	18	1.16
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	7	1.16
(1,176)	1:27:B:ASP:C	1:28:B:LEU:N	1:28:B:LEU:CA	1:28:B:LEU:C	6	1.16
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	8	1.16
(1,40)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:ASN:N	12	1.16
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	1	1.16
(1,17)	1:14:A:SER:C	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	17	1.16
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	6	1.15
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	10	1.15
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	19	1.14
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	11	1.14
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	16	1.14
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	1	1.14
(1,33)	1:23:A:ASP:C	1:24:A:VAL:N	1:24:A:VAL:CA	1:24:A:VAL:C	12	1.14
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	14	1.13
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	14	1.13
(1,93)	1:73:A:THR:C	1:74:A:SER:N	1:74:A:SER:CA	1:74:A:SER:C	7	1.13
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	5	1.12
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	19	1.12
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	15	1.12
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	17	1.12
(1,225)	1:67:B:MET:N	1:67:B:MET:CA	1:67:B:MET:C	1:68:B:LEU:N	1	1.11
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	7	1.11
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	16	1.11
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	4	1.11
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	7	1.11
(1,43)	1:33:A:ASN:C	1:34:A:THR:N	1:34:A:THR:CA	1:34:A:THR:C	11	1.11
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	16	1.11
(1,207)	1:57:B:THR:N	1:57:B:THR:CA	1:57:B:THR:C	1:58:B:ILE:N	8	1.1
(1,176)	1:27:B:ASP:C	1:28:B:LEU:N	1:28:B:LEU:CA	1:28:B:LEU:C	20	1.1
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	13	1.09
(1,108)	1:87:A:LEU:C	1:88:A:SER:N	1:88:A:SER:CA	1:88:A:SER:C	8	1.09
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	6	1.09
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	1	1.09
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	4	1.09
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	14	1.09
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	12	1.08
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	16	1.07
(1,165)	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:C	1:21:B:PHE:N	20	1.07
(1,156)	1:14:B:SER:C	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	15	1.07
(1,55)	1:40:A:LEU:C	1:41:A:THR:N	1:41:A:THR:CA	1:41:A:THR:C	12	1.07
(1,47)	1:35:A:ARG:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	19	1.07
(1,45)	1:34:A:THR:C	1:35:A:ARG:N	1:35:A:ARG:CA	1:35:A:ARG:C	1	1.07
(1,20)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:THR:N	7	1.07
(1,232)	1:73:B:THR:C	1:74:B:SER:N	1:74:B:SER:CA	1:74:B:SER:C	17	1.06
(1,179)	1:30:B:ASP:N	1:30:B:ASP:CA	1:30:B:ASP:C	1:31:B:ASN:N	9	1.06
(1,156)	1:14:B:SER:C	1:15:B:ALA:N	1:15:B:ALA:CA	1:15:B:ALA:C	8	1.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,114)	1:90:A:PHE:C	1:91:A:ARG:N	1:91:A:ARG:CA	1:91:A:ARG:C	7	1.06
(1,51)	1:37:A:VAL:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	14	1.06
(1,47)	1:35:A:ARG:C	1:36:A:LEU:N	1:36:A:LEU:CA	1:36:A:LEU:C	13	1.06
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	20	1.05
(1,165)	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:C	1:21:B:PHE:N	6	1.05
(1,135)	1:101:A:LEU:N	1:101:A:LEU:CA	1:101:A:LEU:C	1:102:A:ILE:N	19	1.05
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	20	1.05
(1,11)	1:11:A:ASP:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	18	1.05
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	5	1.04
(1,190)	1:37:B:VAL:C	1:38:B:ILE:N	1:38:B:ILE:CA	1:38:B:ILE:C	7	1.04
(1,41)	1:30:A:ASP:C	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	10	1.04
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	1	1.04
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	3	1.04
(1,225)	1:67:B:MET:N	1:67:B:MET:CA	1:67:B:MET:C	1:68:B:LEU:N	4	1.03
(1,184)	1:34:B:THR:C	1:35:B:ARG:N	1:35:B:ARG:CA	1:35:B:ARG:C	9	1.03
(1,180)	1:30:B:ASP:C	1:31:B:ASN:N	1:31:B:ASN:CA	1:31:B:ASN:C	10	1.03
(1,176)	1:27:B:ASP:C	1:28:B:LEU:N	1:28:B:LEU:CA	1:28:B:LEU:C	19	1.03
(1,82)	1:65:A:PHE:N	1:65:A:PHE:CA	1:65:A:PHE:C	1:66:A:ILE:N	18	1.03
(1,51)	1:37:A:VAL:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	5	1.03
(1,37)	1:27:A:ASP:C	1:28:A:LEU:N	1:28:A:LEU:CA	1:28:A:LEU:C	11	1.03
(1,247)	1:87:B:LEU:C	1:88:B:SER:N	1:88:B:SER:CA	1:88:B:SER:C	11	1.02
(1,194)	1:40:B:LEU:C	1:41:B:THR:N	1:41:B:THR:CA	1:41:B:THR:C	13	1.02
(1,172)	1:23:B:ASP:C	1:24:B:VAL:N	1:24:B:VAL:CA	1:24:B:VAL:C	5	1.02
(1,170)	1:22:B:VAL:C	1:23:B:ASP:N	1:23:B:ASP:CA	1:23:B:ASP:C	3	1.02
(1,170)	1:22:B:VAL:C	1:23:B:ASP:N	1:23:B:ASP:CA	1:23:B:ASP:C	14	1.02
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	15	1.02
(1,68)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:ILE:N	3	1.02
(1,26)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:PHE:N	14	1.02
(1,227)	1:68:B:LEU:N	1:68:B:LEU:CA	1:68:B:LEU:C	1:69:B:THR:N	8	1.01
(1,210)	1:58:B:ILE:C	1:59:B:HIS:N	1:59:B:HIS:CA	1:59:B:HIS:C	5	1.01
(1,182)	1:33:B:ASN:C	1:34:B:THR:N	1:34:B:THR:CA	1:34:B:THR:C	8	1.01
(1,51)	1:37:A:VAL:C	1:38:A:ILE:N	1:38:A:ILE:CA	1:38:A:ILE:C	16	1.01
(1,11)	1:11:A:ASP:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	17	1.01
(1,253)	1:90:B:PHE:C	1:91:B:ARG:N	1:91:B:ARG:CA	1:91:B:ARG:C	15	1.0
(1,159)	1:16:B:LYS:N	1:16:B:LYS:CA	1:16:B:LYS:C	1:17:B:THR:N	10	1.0