



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 10:27 AM UTC

PDB ID : 2N4X / pdb_00002n4x
BMRB ID : 25685
Title : Structure of the Transmembrane Electron Transporter CcdA
Authors : Chou, J.J.; Williamson, J.A.
Deposited on : 2015-07-01

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

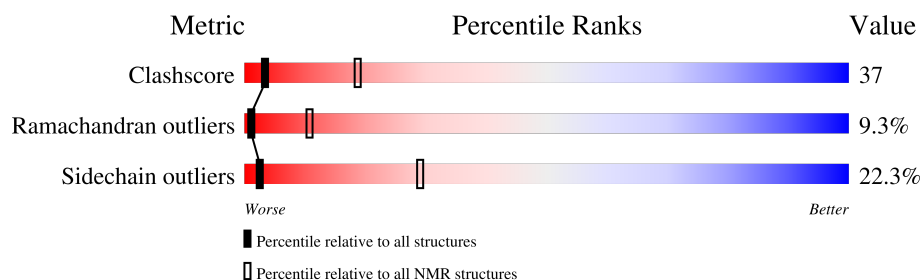
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 30%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	208	22% 49% 5% 16% 8%

2 Ensemble composition and analysis

This entry contains 15 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:17, A:29-A:51, A:57-A:97, A:106-A:184 (158)	1.10	7

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3063 atoms, of which 1584 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytochrome C-type biogenesis protein (CcdA).

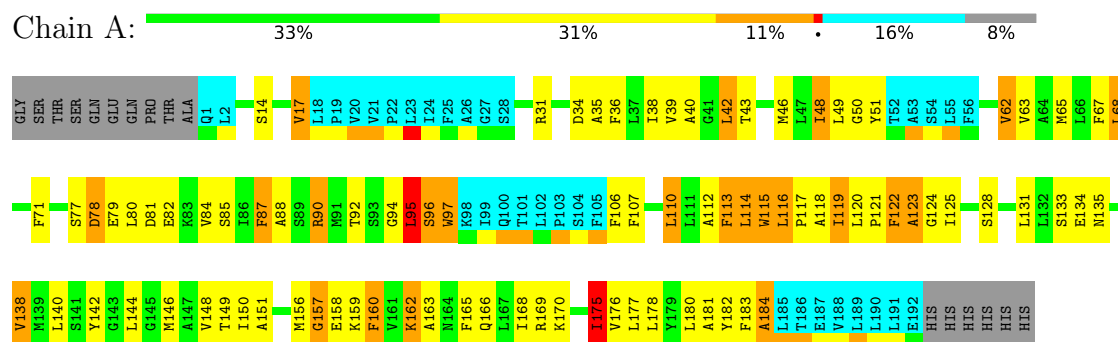
Mol	Chain	Residues	Atoms						Trace
1	A	192	Total	C	H	N	O	S	0
			3063	1008	1584	221	242	8	

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP O29205
A	-8	SER	-	expression tag	UNP O29205
A	-7	THR	-	expression tag	UNP O29205
A	-6	SER	-	expression tag	UNP O29205
A	-5	GLN	-	expression tag	UNP O29205
A	-4	GLU	-	expression tag	UNP O29205
A	-3	GLN	-	expression tag	UNP O29205
A	-2	PRO	-	expression tag	UNP O29205
A	-1	THR	-	expression tag	UNP O29205
A	0	ALA	-	expression tag	UNP O29205
A	1	GLN	-	expression tag	UNP O29205
A	16	ALA	CYS	engineered mutation	UNP O29205
A	118	ALA	CYS	engineered mutation	UNP O29205
A	191	LEU	-	expression tag	UNP O29205
A	192	GLU	-	expression tag	UNP O29205
A	193	HIS	-	expression tag	UNP O29205
A	194	HIS	-	expression tag	UNP O29205
A	195	HIS	-	expression tag	UNP O29205
A	196	HIS	-	expression tag	UNP O29205
A	197	HIS	-	expression tag	UNP O29205
A	198	HIS	-	expression tag	UNP O29205

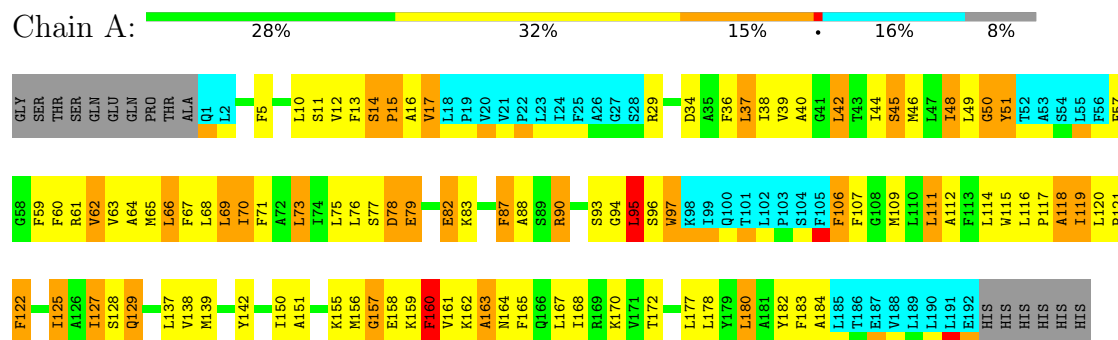
4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



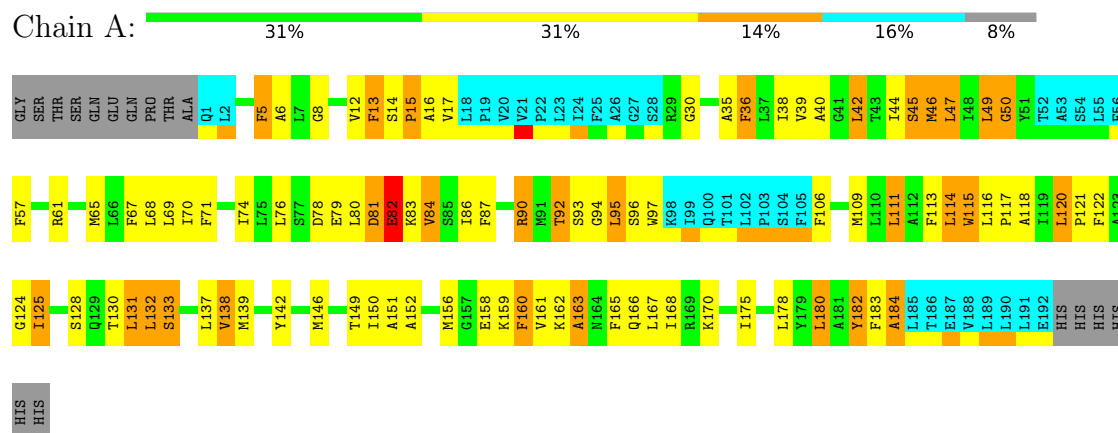
4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



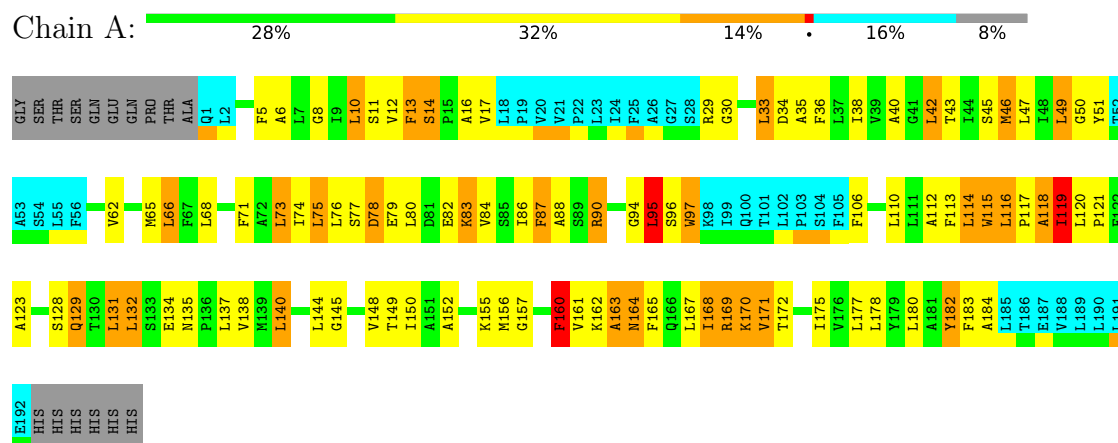
4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



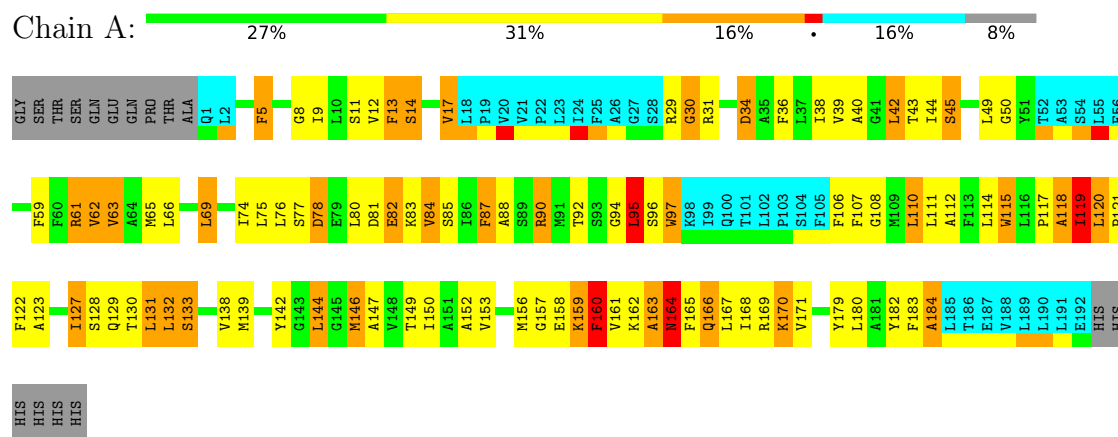
4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



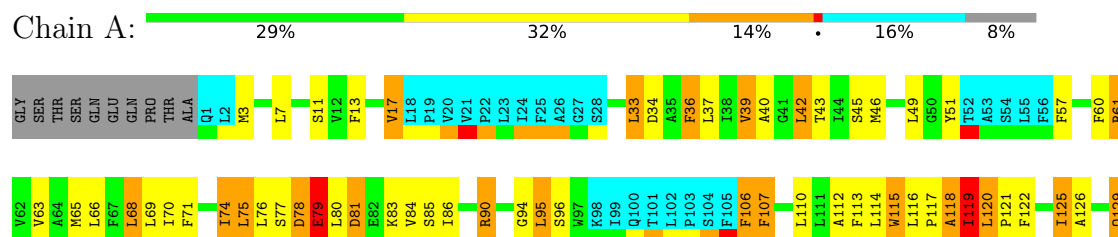
4.2.6 Score per residue for model 6

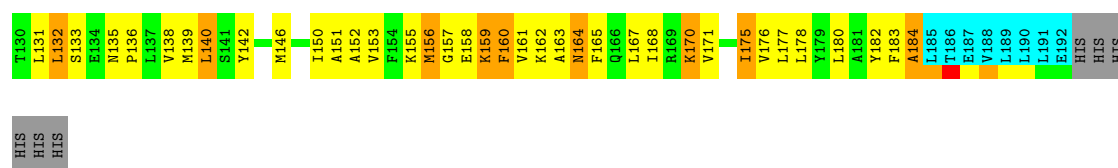
- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



4.2.7 Score per residue for model 7 (medoid)

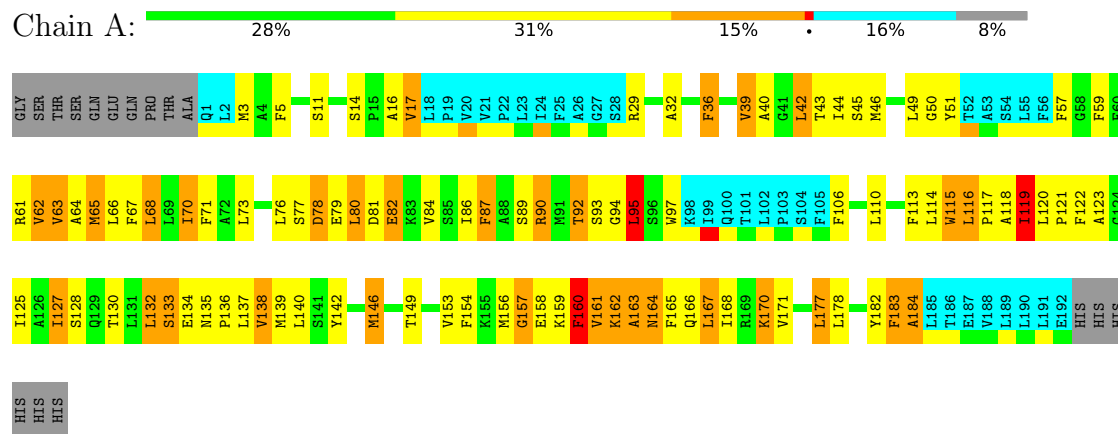
- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)





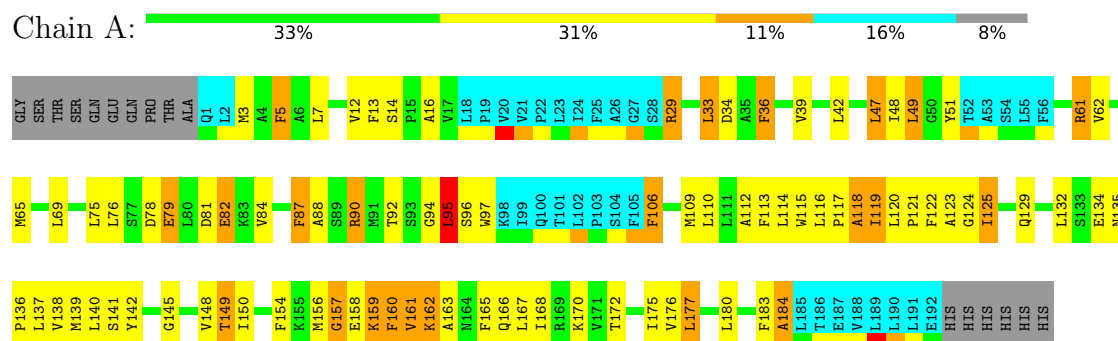
4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



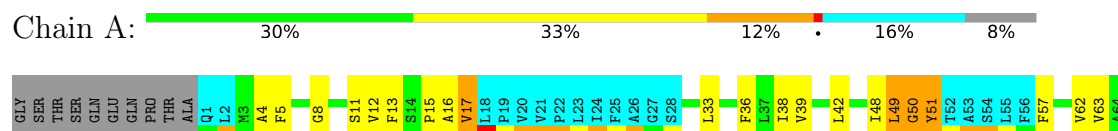
4.2.9 Score per residue for model 9

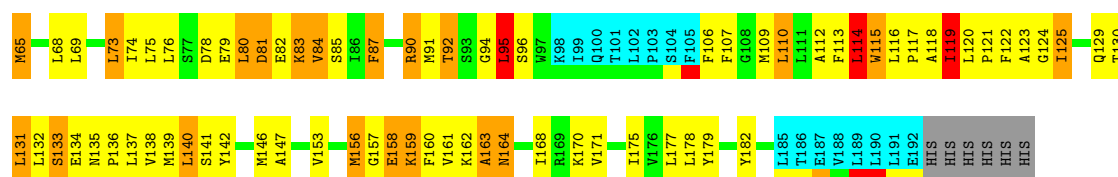
- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



4.2.10 Score per residue for model 10

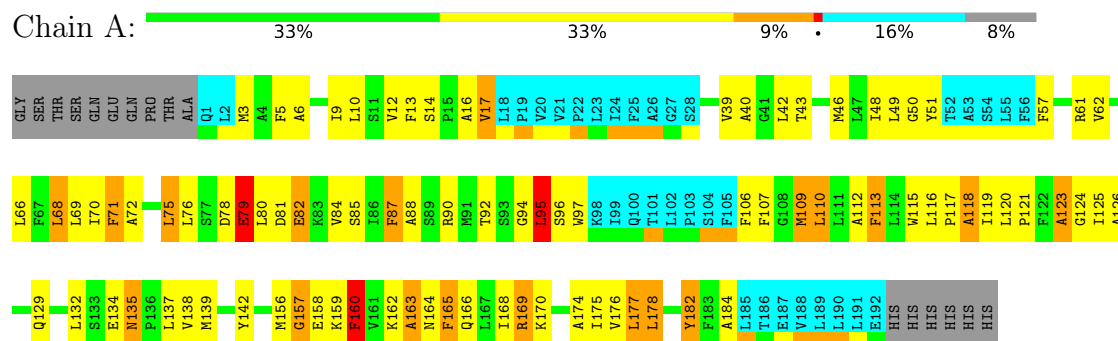
- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)





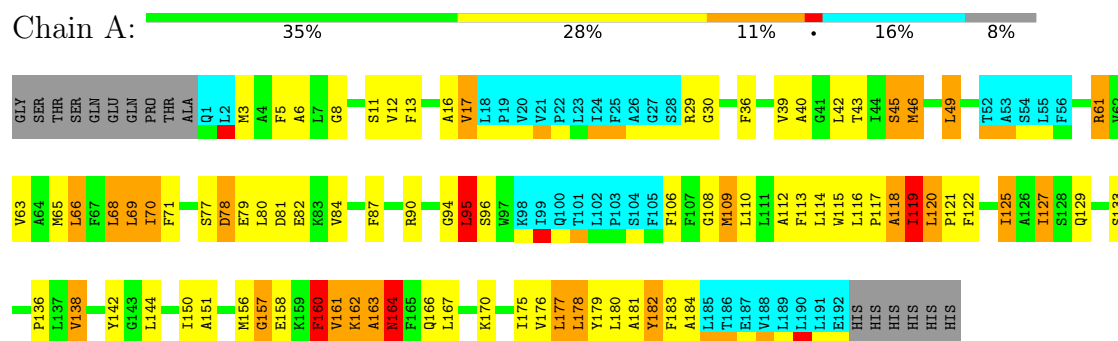
4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



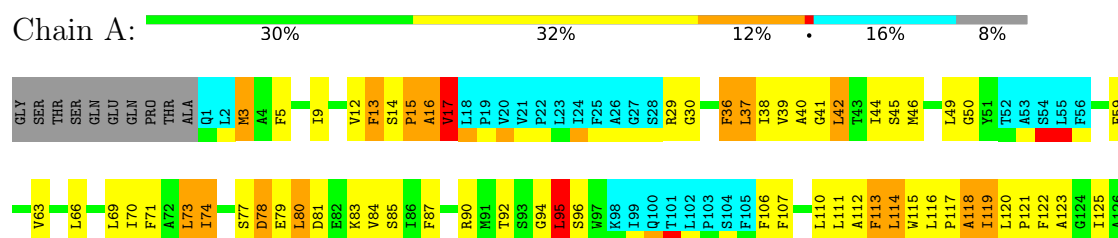
4.2.12 Score per residue for model 12

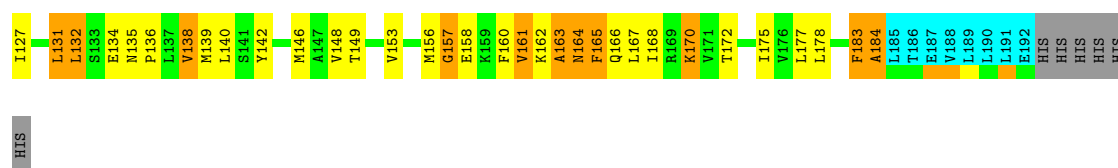
- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



4.2.13 Score per residue for model 13

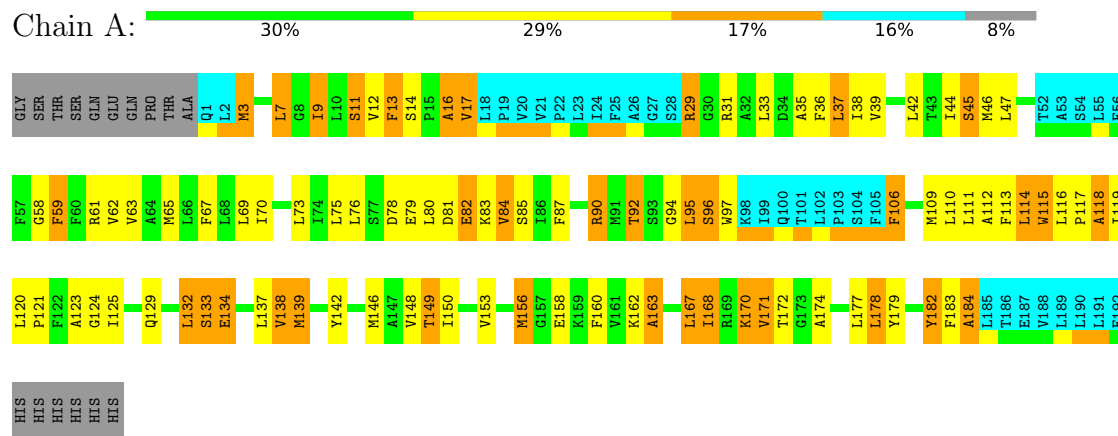
- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)





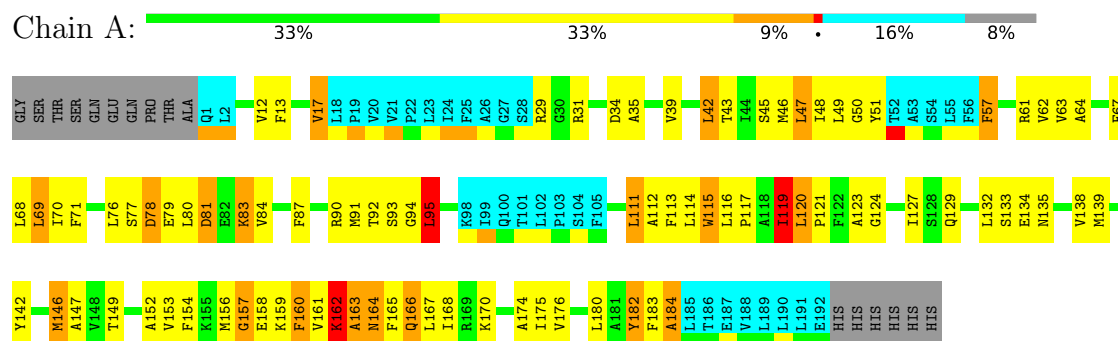
4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome C-type biogenesis protein (CcdA)



5 Refinement protocol and experimental data overview

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

Of the 75 calculated structures, 15 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
X-PLOR NIH	structure solution	2.38
X-PLOR NIH	refinement	2.38

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	765
Number of shifts mapped to atoms	765
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	30%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.01	0±0/1247 (0.0± 0.0%)	1.05±0.02	2±2/1690 (0.1± 0.1%)
All	All	0.73	0/18705 (0.0%)	1.05	32/25350 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	113	PHE	N-CA-C	6.62	118.50	111.28	10	1
1	A	115	TRP	N-CA-C	6.23	118.07	111.28	10	8
1	A	175	ILE	N-CA-C	5.76	116.50	110.62	2	2
1	A	71	PHE	CA-CB-CG	-5.65	108.15	113.80	12	1
1	A	123	ALA	N-CA-C	-5.63	105.14	111.28	11	4
1	A	114	LEU	N-CA-C	5.57	117.35	111.28	2	2
1	A	122	PHE	N-CA-C	-5.48	105.31	111.28	6	3
1	A	113	PHE	CA-CB-CG	-5.42	108.38	113.80	11	2
1	A	176	VAL	N-CA-C	5.32	116.05	110.62	11	2
1	A	146	MET	N-CA-C	5.28	116.84	111.14	6	1
1	A	62	VAL	N-CA-C	5.19	115.41	110.53	2	1
1	A	122	PHE	CA-CB-CG	-5.13	108.67	113.80	2	2
1	A	29	ARG	CB-CA-C	-5.08	109.75	115.79	8	1
1	A	165	PHE	CA-CB-CG	-5.07	108.73	113.80	5	1
1	A	147	ALA	N-CA-C	5.01	116.55	111.14	6	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1218	1299	1299	92±11
All	All	18270	19485	19485	1381

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LEU:HD13	1:A:96:SER:H	0.96	1.21	2	1
1:A:168:ILE:HD13	1:A:169:ARG:N	0.91	1.81	1	1
1:A:127:ILE:HD13	1:A:128:SER:N	0.91	1.79	6	3
1:A:125:ILE:HD13	1:A:126:ALA:N	0.89	1.82	1	2
1:A:95:LEU:HD22	1:A:96:SER:N	0.87	1.85	1	4
1:A:95:LEU:HD12	1:A:96:SER:N	0.83	1.88	5	4
1:A:95:LEU:HD13	1:A:95:LEU:O	0.82	1.74	11	3
1:A:95:LEU:HD13	1:A:96:SER:N	0.81	1.91	2	1
1:A:74:ILE:HD13	1:A:75:LEU:N	0.81	1.91	7	1
1:A:80:LEU:H	1:A:80:LEU:HD13	0.81	1.33	8	1
1:A:92:THR:O	1:A:95:LEU:HD22	0.81	1.76	8	2
1:A:92:THR:O	1:A:95:LEU:HD12	0.80	1.76	2	3
1:A:167:LEU:HD22	1:A:167:LEU:O	0.80	1.77	14	1
1:A:168:ILE:HD13	1:A:169:ARG:H	0.80	1.36	1	1
1:A:95:LEU:HD23	1:A:95:LEU:O	0.78	1.78	8	2
1:A:167:LEU:HD22	1:A:167:LEU:H	0.77	1.40	3	1
1:A:39:VAL:HG12	1:A:117:PRO:O	0.76	1.80	9	12
1:A:68:LEU:HD12	1:A:68:LEU:O	0.75	1.81	12	1
1:A:106:PHE:O	1:A:110:LEU:HD13	0.75	1.81	5	2
1:A:119:ILE:HG22	1:A:120:LEU:N	0.75	1.95	7	10
1:A:161:VAL:HG22	1:A:162:LYS:H	0.74	1.40	3	3
1:A:165:PHE:O	1:A:168:ILE:HD12	0.74	1.82	1	1
1:A:96:SER:HG	1:A:97:TRP:CD1	0.74	2.01	2	1
1:A:167:LEU:HD13	1:A:168:ILE:N	0.73	1.98	14	1
1:A:37:LEU:O	1:A:37:LEU:HD22	0.73	1.84	14	1
1:A:95:LEU:HD12	1:A:95:LEU:C	0.73	2.09	6	5
1:A:177:LEU:C	1:A:177:LEU:HD22	0.73	2.09	11	1
1:A:111:LEU:HD12	1:A:111:LEU:O	0.72	1.83	3	1
1:A:36:PHE:O	1:A:39:VAL:HG22	0.72	1.82	1	10
1:A:33:LEU:C	1:A:33:LEU:HD13	0.72	2.10	5	3
1:A:177:LEU:HD12	1:A:177:LEU:O	0.72	1.83	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:LEU:C	1:A:178:LEU:HD23	0.72	2.10	10	6
1:A:167:LEU:HD22	1:A:167:LEU:C	0.72	2.10	14	1
1:A:120:LEU:H	1:A:120:LEU:HD22	0.71	1.45	14	1
1:A:69:LEU:HD23	1:A:70:ILE:N	0.71	1.99	3	2
1:A:167:LEU:HD22	1:A:167:LEU:N	0.71	2.00	3	1
1:A:115:TRP:O	1:A:175:ILE:HD11	0.70	1.86	4	1
1:A:156:MET:SD	1:A:157:GLY:N	0.70	2.64	10	2
1:A:11:SER:O	1:A:156:MET:HE2	0.70	1.87	5	1
1:A:114:LEU:HD23	1:A:114:LEU:O	0.69	1.87	2	3
1:A:37:LEU:C	1:A:37:LEU:HD13	0.69	2.12	14	1
1:A:132:LEU:C	1:A:132:LEU:HD22	0.69	2.12	6	1
1:A:140:LEU:C	1:A:140:LEU:HD13	0.68	2.14	8	3
1:A:177:LEU:C	1:A:177:LEU:HD13	0.68	2.14	14	1
1:A:122:PHE:O	1:A:125:ILE:HG22	0.66	1.90	10	3
1:A:107:PHE:O	1:A:110:LEU:HD23	0.66	1.91	11	1
1:A:161:VAL:HG22	1:A:162:LYS:N	0.66	2.05	3	6
1:A:87:PHE:CD1	1:A:88:ALA:N	0.66	2.63	5	6
1:A:120:LEU:HD22	1:A:120:LEU:N	0.66	2.06	14	1
1:A:119:ILE:HG22	1:A:120:LEU:H	0.65	1.50	7	3
1:A:17:VAL:O	1:A:17:VAL:HG13	0.65	1.92	6	1
1:A:95:LEU:C	1:A:95:LEU:HD22	0.65	2.15	2	1
1:A:71:PHE:O	1:A:74:ILE:HD12	0.65	1.91	7	1
1:A:95:LEU:HD13	1:A:95:LEU:C	0.65	2.17	1	3
1:A:95:LEU:HD22	1:A:95:LEU:C	0.65	2.16	11	3
1:A:95:LEU:O	1:A:95:LEU:HD12	0.65	1.92	14	1
1:A:68:LEU:HD12	1:A:68:LEU:C	0.65	2.16	12	1
1:A:110:LEU:HD22	1:A:110:LEU:N	0.65	2.07	7	1
1:A:80:LEU:N	1:A:80:LEU:HD12	0.64	2.08	10	1
1:A:90:ARG:CZ	1:A:115:TRP:NE1	0.64	2.60	5	1
1:A:74:ILE:HD13	1:A:75:LEU:H	0.64	1.50	7	1
1:A:114:LEU:O	1:A:114:LEU:HD12	0.64	1.91	14	1
1:A:114:LEU:HD12	1:A:114:LEU:C	0.64	2.17	14	1
1:A:90:ARG:NH2	1:A:179:TYR:CG	0.63	2.66	6	1
1:A:177:LEU:HD12	1:A:178:LEU:N	0.63	2.08	2	1
1:A:107:PHE:CD2	1:A:108:GLY:N	0.63	2.66	6	1
1:A:62:VAL:O	1:A:110:LEU:HD23	0.63	1.94	5	1
1:A:165:PHE:CD1	1:A:166:GLN:N	0.63	2.67	8	2
1:A:122:PHE:CZ	1:A:142:TYR:CE1	0.62	2.86	4	1
1:A:90:ARG:NH1	1:A:115:TRP:NE1	0.62	2.47	7	1
1:A:73:LEU:C	1:A:73:LEU:HD12	0.62	2.19	10	2
1:A:112:ALA:O	1:A:115:TRP:NE1	0.62	2.32	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ALA:HB3	1:A:170:LYS:NZ	0.62	2.09	7	1
1:A:165:PHE:O	1:A:168:ILE:HG22	0.62	1.94	8	3
1:A:90:ARG:NH1	1:A:94:GLY:N	0.62	2.48	13	2
1:A:167:LEU:H	1:A:167:LEU:CD2	0.62	2.08	3	1
1:A:119:ILE:CG2	1:A:120:LEU:N	0.62	2.62	7	8
1:A:95:LEU:HD23	1:A:95:LEU:C	0.61	2.20	8	1
1:A:116:LEU:C	1:A:116:LEU:HD13	0.61	2.20	15	1
1:A:119:ILE:HD11	1:A:175:ILE:HD13	0.61	1.71	2	1
1:A:122:PHE:CE2	1:A:142:TYR:CE2	0.61	2.89	9	2
1:A:112:ALA:O	1:A:115:TRP:CD1	0.61	2.53	12	8
1:A:164:ASN:H	1:A:167:LEU:HD23	0.61	1.54	3	1
1:A:95:LEU:HD22	1:A:96:SER:O	0.61	1.95	2	1
1:A:138:VAL:O	1:A:142:TYR:CG	0.61	2.54	6	7
1:A:115:TRP:CD1	1:A:116:LEU:N	0.60	2.69	4	5
1:A:125:ILE:CD1	1:A:129:GLN:NE2	0.60	2.64	3	1
1:A:156:MET:SD	1:A:160:PHE:CE2	0.60	2.94	3	2
1:A:169:ARG:O	1:A:172:THR:HG22	0.60	1.95	5	1
1:A:106:PHE:CD2	1:A:109:MET:SD	0.60	2.95	4	1
1:A:49:LEU:O	1:A:49:LEU:HD23	0.60	1.96	13	1
1:A:49:LEU:HD13	1:A:49:LEU:C	0.60	2.21	7	1
1:A:90:ARG:HE	1:A:90:ARG:C	0.60	2.05	14	2
1:A:69:LEU:C	1:A:69:LEU:HD23	0.60	2.22	12	2
1:A:90:ARG:HH22	1:A:94:GLY:CA	0.60	2.10	14	1
1:A:69:LEU:HD13	1:A:69:LEU:O	0.60	1.96	15	1
1:A:46:MET:SD	1:A:46:MET:N	0.60	2.74	5	2
1:A:117:PRO:O	1:A:118:ALA:O	0.60	2.19	12	7
1:A:122:PHE:CZ	1:A:177:LEU:HD13	0.60	2.32	2	1
1:A:37:LEU:HD13	1:A:38:ILE:N	0.60	2.12	14	1
1:A:110:LEU:O	1:A:113:PHE:CE1	0.59	2.55	2	1
1:A:14:SER:O	1:A:156:MET:HE2	0.59	1.97	6	1
1:A:146:MET:SD	1:A:146:MET:N	0.59	2.75	8	1
1:A:49:LEU:O	1:A:51:TYR:N	0.59	2.35	15	6
1:A:106:PHE:CG	1:A:109:MET:SD	0.59	2.96	9	1
1:A:15:PRO:O	1:A:16:ALA:HB3	0.59	1.98	1	2
1:A:120:LEU:O	1:A:123:ALA:HB3	0.59	1.97	6	9
1:A:90:ARG:HH11	1:A:115:TRP:CD1	0.59	2.15	6	1
1:A:153:VAL:O	1:A:156:MET:SD	0.59	2.61	10	2
1:A:141:SER:OG	1:A:177:LEU:HD21	0.59	1.97	9	1
1:A:77:SER:O	1:A:79:GLU:N	0.59	2.36	3	1
1:A:152:ALA:HB3	1:A:167:LEU:HD21	0.59	1.74	6	1
1:A:120:LEU:N	1:A:121:PRO:HD2	0.59	2.12	2	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:164:ASN:ND2	1:A:166:GLN:H	0.59	1.95	12	1
1:A:65:MET:SD	1:A:65:MET:N	0.58	2.75	8	2
1:A:90:ARG:HH12	1:A:94:GLY:N	0.58	1.95	13	2
1:A:80:LEU:HD12	1:A:80:LEU:H	0.58	1.57	10	1
1:A:109:MET:SD	1:A:109:MET:N	0.58	2.76	10	2
1:A:137:LEU:N	1:A:137:LEU:HD23	0.58	2.13	4	1
1:A:46:MET:SD	1:A:61:ARG:NH2	0.58	2.76	12	1
1:A:178:LEU:HD23	1:A:178:LEU:O	0.58	1.98	4	4
1:A:156:MET:SD	1:A:160:PHE:CD2	0.58	2.96	3	1
1:A:86:ILE:N	1:A:86:ILE:HD12	0.58	2.12	4	2
1:A:167:LEU:HD12	1:A:167:LEU:N	0.58	2.14	9	1
1:A:116:LEU:HD12	1:A:116:LEU:H	0.58	1.58	9	2
1:A:122:PHE:CE2	1:A:142:TYR:CE1	0.58	2.91	10	1
1:A:127:ILE:HD13	1:A:128:SER:H	0.58	1.59	6	2
1:A:39:VAL:CG1	1:A:117:PRO:O	0.58	2.51	9	14
1:A:90:ARG:CZ	1:A:115:TRP:CD1	0.58	2.86	14	2
1:A:156:MET:O	1:A:158:GLU:N	0.58	2.37	3	12
1:A:165:PHE:CD1	1:A:165:PHE:C	0.58	2.82	9	5
1:A:109:MET:SD	1:A:113:PHE:CZ	0.57	2.97	12	1
1:A:36:PHE:CD1	1:A:37:LEU:N	0.57	2.72	7	1
1:A:33:LEU:HD12	1:A:34:ASP:N	0.57	2.14	9	1
1:A:65:MET:SD	1:A:114:LEU:HD21	0.57	2.39	9	1
1:A:164:ASN:HD22	1:A:166:GLN:H	0.57	1.42	12	1
1:A:48:ILE:HD12	1:A:61:ARG:HH21	0.57	1.59	3	1
1:A:112:ALA:O	1:A:115:TRP:CE2	0.57	2.57	13	5
1:A:12:VAL:O	1:A:14:SER:N	0.57	2.37	6	5
1:A:87:PHE:CE2	1:A:115:TRP:CZ2	0.57	2.92	4	1
1:A:127:ILE:HD12	1:A:127:ILE:N	0.57	2.15	13	1
1:A:83:LYS:NZ	1:A:172:THR:OG1	0.57	2.37	3	1
1:A:111:LEU:HD12	1:A:111:LEU:C	0.57	2.25	3	1
1:A:164:ASN:N	1:A:167:LEU:HD23	0.57	2.15	3	1
1:A:35:ALA:O	1:A:38:ILE:HG22	0.57	2.00	14	3
1:A:90:ARG:NH1	1:A:94:GLY:CA	0.57	2.68	1	2
1:A:90:ARG:CB	1:A:115:TRP:CZ3	0.57	2.88	10	2
1:A:33:LEU:HD22	1:A:33:LEU:N	0.57	2.14	14	1
1:A:64:ALA:O	1:A:67:PHE:CD2	0.57	2.58	3	2
1:A:33:LEU:HD13	1:A:34:ASP:N	0.57	2.15	7	2
1:A:83:LYS:NZ	1:A:168:ILE:HD12	0.57	2.15	10	1
1:A:49:LEU:N	1:A:61:ARG:HH21	0.57	1.97	11	1
1:A:162:LYS:O	1:A:163:ALA:HB2	0.57	2.00	14	6
1:A:46:MET:SD	1:A:61:ARG:CZ	0.56	2.93	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:O	1:A:117:PRO:HD2	0.56	2.00	6	9
1:A:120:LEU:N	1:A:121:PRO:CD	0.56	2.68	15	5
1:A:66:LEU:HD22	1:A:66:LEU:N	0.56	2.15	11	3
1:A:76:LEU:N	1:A:76:LEU:HD12	0.56	2.15	3	4
1:A:57:PHE:O	1:A:61:ARG:NH2	0.56	2.38	7	1
1:A:138:VAL:HG23	1:A:139:MET:N	0.56	2.16	10	4
1:A:116:LEU:HD13	1:A:116:LEU:O	0.56	2.01	15	1
1:A:90:ARG:O	1:A:90:ARG:NE	0.56	2.39	2	5
1:A:42:LEU:O	1:A:46:MET:SD	0.56	2.64	13	2
1:A:132:LEU:HD13	1:A:133:SER:H	0.56	1.61	4	1
1:A:76:LEU:HD22	1:A:76:LEU:N	0.56	2.16	5	2
1:A:162:LYS:O	1:A:163:ALA:CB	0.55	2.54	3	4
1:A:129:GLN:N	1:A:129:GLN:OE1	0.55	2.39	5	1
1:A:90:ARG:NH1	1:A:93:SER:OG	0.55	2.40	1	1
1:A:81:ASP:OD1	1:A:82:GLU:N	0.55	2.40	2	1
1:A:109:MET:O	1:A:113:PHE:CD1	0.55	2.60	9	1
1:A:120:LEU:H	1:A:120:LEU:CD2	0.55	2.13	14	1
1:A:110:LEU:O	1:A:113:PHE:CD1	0.55	2.59	2	1
1:A:33:LEU:HD22	1:A:33:LEU:O	0.55	2.00	7	2
1:A:132:LEU:H	1:A:132:LEU:CD1	0.55	2.14	6	1
1:A:90:ARG:NH1	1:A:115:TRP:CE2	0.55	2.74	7	1
1:A:15:PRO:O	1:A:16:ALA:CB	0.55	2.55	13	2
1:A:34:ASP:OD1	1:A:35:ALA:N	0.55	2.40	2	2
1:A:84:VAL:HG23	1:A:85:SER:N	0.55	2.17	11	4
1:A:92:THR:O	1:A:95:LEU:HD11	0.55	2.00	14	1
1:A:161:VAL:HG13	1:A:162:LYS:N	0.55	2.17	9	2
1:A:156:MET:C	1:A:156:MET:SD	0.55	2.90	5	3
1:A:45:SER:O	1:A:61:ARG:NH2	0.55	2.40	4	2
1:A:70:ILE:HD13	1:A:70:ILE:O	0.55	2.02	3	3
1:A:138:VAL:O	1:A:142:TYR:CD1	0.55	2.60	13	5
1:A:78:ASP:OD1	1:A:79:GLU:N	0.54	2.40	15	3
1:A:80:LEU:HD22	1:A:80:LEU:N	0.54	2.17	15	2
1:A:68:LEU:O	1:A:68:LEU:HD13	0.54	2.01	2	1
1:A:110:LEU:N	1:A:110:LEU:CD2	0.54	2.70	7	1
1:A:83:LYS:NZ	1:A:168:ILE:CD1	0.54	2.70	15	2
1:A:42:LEU:HD12	1:A:42:LEU:O	0.54	2.02	6	1
1:A:49:LEU:HD13	1:A:49:LEU:O	0.54	2.02	7	1
1:A:94:GLY:O	1:A:96:SER:N	0.54	2.40	2	1
1:A:116:LEU:HD23	1:A:116:LEU:O	0.54	2.03	5	1
1:A:82:GLU:H	1:A:82:GLU:CD	0.54	2.10	6	4
1:A:166:GLN:HE21	1:A:166:GLN:C	0.54	2.11	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ILE:HG22	1:A:61:ARG:NH2	0.54	2.17	11	1
1:A:90:ARG:NH2	1:A:94:GLY:N	0.54	2.56	14	1
1:A:5:PHE:CD1	1:A:6:ALA:N	0.54	2.75	11	3
1:A:65:MET:CE	1:A:114:LEU:HD21	0.54	2.33	9	1
1:A:132:LEU:CD2	1:A:132:LEU:H	0.54	2.16	10	1
1:A:79:GLU:H	1:A:79:GLU:CD	0.54	2.10	1	1
1:A:8:GLY:O	1:A:36:PHE:CE2	0.54	2.61	12	2
1:A:82:GLU:C	1:A:84:VAL:H	0.54	2.10	12	5
1:A:90:ARG:NH1	1:A:115:TRP:CD1	0.54	2.76	6	1
1:A:167:LEU:N	1:A:167:LEU:CD2	0.54	2.71	3	1
1:A:80:LEU:N	1:A:80:LEU:CD2	0.54	2.71	13	3
1:A:62:VAL:O	1:A:65:MET:SD	0.54	2.65	10	1
1:A:125:ILE:HG21	1:A:142:TYR:OH	0.53	2.02	10	2
1:A:138:VAL:HG13	1:A:139:MET:N	0.53	2.17	9	3
1:A:69:LEU:HD23	1:A:113:PHE:CZ	0.53	2.39	15	1
1:A:12:VAL:O	1:A:13:PHE:C	0.53	2.52	5	12
1:A:95:LEU:O	1:A:96:SER:O	0.53	2.27	2	1
1:A:180:LEU:N	1:A:180:LEU:CD2	0.53	2.71	7	9
1:A:146:MET:SD	1:A:147:ALA:N	0.53	2.82	15	2
1:A:90:ARG:NH2	1:A:176:VAL:O	0.53	2.41	12	1
1:A:45:SER:O	1:A:61:ARG:NE	0.53	2.41	3	2
1:A:145:GLY:O	1:A:149:THR:HG22	0.53	2.02	5	1
1:A:11:SER:O	1:A:156:MET:SD	0.53	2.67	14	2
1:A:106:PHE:O	1:A:110:LEU:HD23	0.53	2.03	9	1
1:A:79:GLU:CD	1:A:80:LEU:N	0.53	2.67	4	1
1:A:59:PHE:CD1	1:A:59:PHE:C	0.53	2.86	14	2
1:A:149:THR:HG22	1:A:170:LYS:HB2	0.53	1.80	15	1
1:A:62:VAL:CG2	1:A:110:LEU:HD23	0.53	2.34	2	1
1:A:66:LEU:N	1:A:66:LEU:CD2	0.53	2.71	11	3
1:A:69:LEU:O	1:A:69:LEU:HD23	0.53	2.04	6	2
1:A:80:LEU:HD23	1:A:80:LEU:N	0.53	2.19	7	1
1:A:137:LEU:HD12	1:A:137:LEU:N	0.53	2.19	1	3
1:A:168:ILE:CD1	1:A:169:ARG:N	0.53	2.68	1	1
1:A:152:ALA:HB3	1:A:170:LYS:HZ1	0.53	1.62	7	1
1:A:156:MET:C	1:A:158:GLU:N	0.53	2.65	4	12
1:A:106:PHE:CD1	1:A:109:MET:SD	0.53	3.02	9	1
1:A:79:GLU:OE1	1:A:79:GLU:N	0.53	2.42	11	1
1:A:90:ARG:NH2	1:A:90:ARG:O	0.53	2.42	14	1
1:A:64:ALA:O	1:A:67:PHE:CE2	0.53	2.62	8	1
1:A:164:ASN:CG	1:A:165:PHE:N	0.52	2.67	3	1
1:A:76:LEU:N	1:A:76:LEU:CD2	0.52	2.72	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LEU:O	1:A:50:GLY:C	0.52	2.52	10	7
1:A:87:PHE:C	1:A:87:PHE:CD1	0.52	2.87	1	5
1:A:68:LEU:N	1:A:68:LEU:HD22	0.52	2.20	15	1
1:A:113:PHE:CD1	1:A:113:PHE:N	0.52	2.75	15	7
1:A:148:VAL:HG23	1:A:149:THR:N	0.52	2.19	2	3
1:A:161:VAL:CG2	1:A:162:LYS:H	0.52	2.16	3	2
1:A:70:ILE:HD12	1:A:70:ILE:N	0.52	2.18	14	1
1:A:166:GLN:C	1:A:166:GLN:NE2	0.52	2.68	6	1
1:A:81:ASP:O	1:A:82:GLU:O	0.52	2.27	8	1
1:A:161:VAL:HG11	1:A:164:ASN:OD1	0.52	2.05	7	2
1:A:33:LEU:HD13	1:A:33:LEU:O	0.52	2.03	10	1
1:A:36:PHE:C	1:A:36:PHE:CD1	0.52	2.88	13	1
1:A:178:LEU:C	1:A:178:LEU:CD2	0.52	2.83	1	6
1:A:109:MET:O	1:A:113:PHE:CE1	0.52	2.62	4	1
1:A:90:ARG:NE	1:A:115:TRP:NE1	0.52	2.58	5	1
1:A:161:VAL:HG21	1:A:164:ASN:OD1	0.52	2.05	7	1
1:A:33:LEU:HD12	1:A:34:ASP:H	0.52	1.64	9	1
1:A:48:ILE:C	1:A:61:ARG:NH2	0.52	2.67	11	1
1:A:161:VAL:O	1:A:162:LYS:CB	0.52	2.56	15	1
1:A:82:GLU:O	1:A:84:VAL:N	0.52	2.42	10	5
1:A:33:LEU:C	1:A:33:LEU:CD1	0.52	2.82	5	3
1:A:134:GLU:CD	1:A:134:GLU:N	0.52	2.68	9	1
1:A:50:GLY:O	1:A:51:TYR:CB	0.52	2.57	3	1
1:A:90:ARG:NE	1:A:93:SER:OG	0.52	2.43	3	1
1:A:90:ARG:NH2	1:A:179:TYR:CD2	0.52	2.77	6	1
1:A:168:ILE:O	1:A:171:VAL:HG12	0.52	2.04	7	1
1:A:82:GLU:N	1:A:82:GLU:OE1	0.52	2.42	11	1
1:A:37:LEU:C	1:A:37:LEU:CD1	0.52	2.83	14	1
1:A:138:VAL:CG2	1:A:139:MET:N	0.52	2.72	1	7
1:A:168:ILE:O	1:A:171:VAL:HG22	0.52	2.04	14	2
1:A:139:MET:C	1:A:139:MET:SD	0.52	2.93	10	2
1:A:122:PHE:CZ	1:A:142:TYR:CZ	0.52	2.98	7	2
1:A:5:PHE:C	1:A:5:PHE:CD1	0.52	2.88	6	3
1:A:14:SER:CB	1:A:156:MET:O	0.52	2.58	4	4
1:A:128:SER:O	1:A:131:LEU:HD12	0.52	2.05	5	1
1:A:132:LEU:C	1:A:132:LEU:CD2	0.52	2.83	6	1
1:A:149:THR:HG23	1:A:167:LEU:CD2	0.52	2.34	8	1
1:A:96:SER:OG	1:A:97:TRP:N	0.52	2.42	9	2
1:A:149:THR:OG1	1:A:170:LYS:CE	0.51	2.58	2	2
1:A:82:GLU:N	1:A:82:GLU:CD	0.51	2.68	3	1
1:A:158:GLU:N	1:A:158:GLU:CD	0.51	2.68	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:ILE:HG21	1:A:142:TYR:CZ	0.51	2.40	4	2
1:A:44:ILE:HD12	1:A:44:ILE:N	0.51	2.20	6	1
1:A:135:ASN:O	1:A:139:MET:SD	0.51	2.68	8	1
1:A:48:ILE:CD1	1:A:61:ARG:HH21	0.51	2.18	3	1
1:A:67:PHE:C	1:A:67:PHE:CD1	0.51	2.87	3	2
1:A:46:MET:CE	1:A:182:TYR:CD2	0.51	2.93	8	1
1:A:141:SER:O	1:A:144:LEU:CD2	0.51	2.59	1	1
1:A:90:ARG:HH21	1:A:94:GLY:CA	0.51	2.18	8	2
1:A:137:LEU:CD2	1:A:137:LEU:H	0.51	2.19	4	1
1:A:80:LEU:H	1:A:80:LEU:CD1	0.51	2.18	10	1
1:A:161:VAL:HG21	1:A:164:ASN:ND2	0.51	2.19	1	1
1:A:139:MET:SD	1:A:139:MET:O	0.51	2.68	10	1
1:A:122:PHE:CD1	1:A:178:LEU:HD12	0.51	2.40	12	1
1:A:161:VAL:HG13	1:A:162:LYS:H	0.51	1.65	9	2
1:A:67:PHE:O	1:A:67:PHE:CD1	0.51	2.64	14	1
1:A:60:PHE:C	1:A:60:PHE:CD1	0.51	2.88	3	2
1:A:132:LEU:HD13	1:A:133:SER:N	0.51	2.20	8	1
1:A:150:ILE:CG2	1:A:154:PHE:CE1	0.51	2.93	9	1
1:A:82:GLU:O	1:A:84:VAL:HG13	0.51	2.05	10	1
1:A:46:MET:SD	1:A:182:TYR:OH	0.51	2.67	11	2
1:A:174:ALA:O	1:A:177:LEU:CD1	0.51	2.59	11	1
1:A:163:ALA:O	1:A:164:ASN:C	0.51	2.53	8	3
1:A:69:LEU:HD12	1:A:113:PHE:CZ	0.51	2.40	12	1
1:A:179:TYR:C	1:A:179:TYR:CD1	0.51	2.88	14	1
1:A:48:ILE:O	1:A:48:ILE:HD13	0.51	2.06	2	1
1:A:129:GLN:OE1	1:A:139:MET:SD	0.51	2.68	9	1
1:A:68:LEU:N	1:A:68:LEU:CD2	0.51	2.74	15	1
1:A:82:GLU:O	1:A:85:SER:N	0.51	2.44	1	2
1:A:91:MET:C	1:A:91:MET:SD	0.51	2.94	1	2
1:A:82:GLU:C	1:A:84:VAL:N	0.51	2.67	14	6
1:A:115:TRP:CD1	1:A:116:LEU:H	0.51	2.22	10	2
1:A:78:ASP:CG	1:A:79:GLU:N	0.51	2.69	9	3
1:A:110:LEU:CD2	1:A:110:LEU:H	0.51	2.19	7	1
1:A:137:LEU:CD2	1:A:137:LEU:N	0.51	2.73	14	3
1:A:82:GLU:CD	1:A:82:GLU:H	0.51	2.13	3	1
1:A:137:LEU:O	1:A:137:LEU:HD23	0.51	2.06	3	1
1:A:17:VAL:O	1:A:17:VAL:CG1	0.50	2.59	6	1
1:A:129:GLN:OE1	1:A:142:TYR:CG	0.50	2.64	10	1
1:A:46:MET:SD	1:A:46:MET:C	0.50	2.94	11	1
1:A:164:ASN:HD22	1:A:164:ASN:C	0.50	2.15	12	1
1:A:149:THR:HG23	1:A:167:LEU:HD21	0.50	1.83	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:C	1:A:68:LEU:CD1	0.50	2.83	12	1
1:A:146:MET:C	1:A:146:MET:SD	0.50	2.94	1	6
1:A:149:THR:OG1	1:A:170:LYS:CB	0.50	2.59	8	2
1:A:42:LEU:HD21	1:A:118:ALA:HB2	0.50	1.83	5	1
1:A:61:ARG:O	1:A:65:MET:SD	0.50	2.69	8	1
1:A:48:ILE:HD12	1:A:61:ARG:CZ	0.50	2.35	9	1
1:A:95:LEU:C	1:A:95:LEU:CD1	0.50	2.80	6	8
1:A:49:LEU:C	1:A:51:TYR:N	0.50	2.68	2	3
1:A:11:SER:OG	1:A:36:PHE:CZ	0.50	2.64	12	1
1:A:45:SER:CB	1:A:61:ARG:HH11	0.50	2.19	15	1
1:A:111:LEU:O	1:A:111:LEU:HD13	0.50	2.07	15	1
1:A:90:ARG:HH12	1:A:94:GLY:CA	0.50	2.20	1	1
1:A:150:ILE:HG23	1:A:151:ALA:N	0.50	2.21	12	4
1:A:161:VAL:CG2	1:A:162:LYS:N	0.50	2.75	6	6
1:A:36:PHE:CZ	1:A:120:LEU:HD13	0.50	2.40	2	1
1:A:149:THR:OG1	1:A:170:LYS:CG	0.50	2.59	8	1
1:A:137:LEU:N	1:A:137:LEU:HD22	0.50	2.21	14	3
1:A:11:SER:OG	1:A:36:PHE:CE2	0.50	2.64	12	1
1:A:14:SER:OG	1:A:156:MET:SD	0.50	2.67	5	2
1:A:90:ARG:NH1	1:A:179:TYR:CB	0.50	2.74	14	1
1:A:142:TYR:CE1	1:A:177:LEU:HD11	0.50	2.41	14	1
1:A:149:THR:HG23	1:A:150:ILE:N	0.50	2.22	5	4
1:A:106:PHE:O	1:A:108:GLY:N	0.50	2.42	12	1
1:A:77:SER:O	1:A:78:ASP:O	0.49	2.30	8	5
1:A:160:PHE:O	1:A:161:VAL:O	0.49	2.29	13	2
1:A:92:THR:O	1:A:95:LEU:CD1	0.49	2.59	14	1
1:A:146:MET:SD	1:A:146:MET:C	0.49	2.94	15	1
1:A:73:LEU:O	1:A:73:LEU:HD13	0.49	2.07	5	2
1:A:156:MET:O	1:A:157:GLY:C	0.49	2.55	3	12
1:A:34:ASP:O	1:A:37:LEU:CD1	0.49	2.60	3	1
1:A:67:PHE:O	1:A:70:ILE:HG22	0.49	2.07	4	1
1:A:80:LEU:H	1:A:80:LEU:CD2	0.49	2.20	7	1
1:A:5:PHE:CD1	1:A:5:PHE:C	0.49	2.90	9	3
1:A:160:PHE:O	1:A:161:VAL:HG12	0.49	2.07	12	1
1:A:75:LEU:HD13	1:A:75:LEU:O	0.49	2.07	11	3
1:A:8:GLY:C	1:A:36:PHE:CE1	0.49	2.90	6	1
1:A:116:LEU:O	1:A:116:LEU:HD13	0.49	2.07	8	1
1:A:116:LEU:N	1:A:117:PRO:HD2	0.49	2.23	4	6
1:A:9:ILE:CD1	1:A:36:PHE:CD2	0.49	2.96	6	1
1:A:178:LEU:HD23	1:A:179:TYR:N	0.49	2.23	10	2
1:A:132:LEU:HD22	1:A:133:SER:N	0.49	2.22	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:ARG:HE	1:A:169:ARG:C	0.49	2.16	11	1
1:A:82:GLU:CD	1:A:82:GLU:N	0.49	2.71	9	3
1:A:183:PHE:O	1:A:184:ALA:C	0.49	2.56	14	11
1:A:5:PHE:CG	1:A:6:ALA:N	0.49	2.80	5	3
1:A:37:LEU:HD23	1:A:37:LEU:O	0.49	2.07	13	2
1:A:138:VAL:CG1	1:A:139:MET:N	0.49	2.75	11	3
1:A:39:VAL:HG13	1:A:117:PRO:O	0.49	2.07	15	1
1:A:57:PHE:O	1:A:61:ARG:NH1	0.49	2.46	1	2
1:A:139:MET:O	1:A:143:GLY:N	0.49	2.45	1	1
1:A:156:MET:C	1:A:158:GLU:H	0.49	2.15	2	4
1:A:42:LEU:HD12	1:A:42:LEU:C	0.49	2.32	6	2
1:A:46:MET:CG	1:A:182:TYR:CZ	0.49	2.96	12	3
1:A:142:TYR:O	1:A:146:MET:SD	0.49	2.70	8	1
1:A:127:ILE:HD12	1:A:127:ILE:H	0.49	1.67	13	1
1:A:177:LEU:C	1:A:177:LEU:CD1	0.49	2.86	14	1
1:A:140:LEU:C	1:A:140:LEU:CD1	0.49	2.85	8	3
1:A:86:ILE:N	1:A:86:ILE:CD1	0.49	2.76	7	2
1:A:42:LEU:CD2	1:A:118:ALA:HB2	0.49	2.37	6	1
1:A:7:LEU:N	1:A:7:LEU:CD2	0.49	2.75	7	1
1:A:122:PHE:CZ	1:A:142:TYR:OH	0.49	2.66	7	2
1:A:74:ILE:HD13	1:A:74:ILE:O	0.49	2.07	13	1
1:A:76:LEU:N	1:A:76:LEU:CD1	0.48	2.76	4	3
1:A:84:VAL:CG2	1:A:85:SER:N	0.48	2.76	11	6
1:A:137:LEU:N	1:A:137:LEU:CD1	0.48	2.76	5	2
1:A:94:GLY:O	1:A:95:LEU:C	0.48	2.55	2	13
1:A:180:LEU:N	1:A:180:LEU:HD22	0.48	2.23	2	5
1:A:48:ILE:HD12	1:A:61:ARG:NH2	0.48	2.23	3	2
1:A:137:LEU:HD23	1:A:137:LEU:H	0.48	1.66	4	1
1:A:170:LYS:HB2	1:A:170:LYS:NZ	0.48	2.22	14	1
1:A:7:LEU:N	1:A:7:LEU:HD22	0.48	2.22	7	1
1:A:80:LEU:N	1:A:80:LEU:CD1	0.48	2.76	10	1
1:A:156:MET:SD	1:A:160:PHE:CZ	0.48	3.06	12	1
1:A:77:SER:O	1:A:78:ASP:C	0.48	2.57	12	10
1:A:16:ALA:O	1:A:17:VAL:O	0.48	2.30	11	5
1:A:94:GLY:O	1:A:95:LEU:O	0.48	2.32	9	9
1:A:49:LEU:O	1:A:49:LEU:HD13	0.48	2.07	4	2
1:A:150:ILE:O	1:A:150:ILE:HD13	0.48	2.08	1	1
1:A:10:LEU:HD13	1:A:10:LEU:O	0.48	2.09	5	1
1:A:44:ILE:N	1:A:44:ILE:CD1	0.48	2.76	6	1
1:A:132:LEU:N	1:A:132:LEU:HD13	0.48	2.24	6	1
1:A:33:LEU:N	1:A:33:LEU:CD2	0.48	2.76	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:TRP:CE3	1:A:175:ILE:HD11	0.48	2.43	15	1
1:A:47:LEU:O	1:A:47:LEU:HD13	0.48	2.08	9	3
1:A:179:TYR:CD1	1:A:179:TYR:O	0.48	2.67	14	1
1:A:9:ILE:HD13	1:A:9:ILE:O	0.48	2.09	14	1
1:A:69:LEU:HD12	1:A:69:LEU:N	0.48	2.23	14	1
1:A:78:ASP:CG	1:A:79:GLU:H	0.48	2.15	5	3
1:A:121:PRO:O	1:A:124:GLY:N	0.48	2.47	11	7
1:A:167:LEU:N	1:A:167:LEU:CD1	0.48	2.76	9	1
1:A:78:ASP:O	1:A:79:GLU:C	0.48	2.57	3	2
1:A:80:LEU:HD23	1:A:81:ASP:N	0.48	2.24	6	1
1:A:122:PHE:O	1:A:142:TYR:OH	0.48	2.28	9	1
1:A:69:LEU:O	1:A:73:LEU:HD23	0.48	2.09	13	1
1:A:114:LEU:C	1:A:114:LEU:CD1	0.48	2.84	14	1
1:A:140:LEU:O	1:A:140:LEU:HD13	0.48	2.09	7	3
1:A:106:PHE:O	1:A:110:LEU:CD2	0.48	2.62	9	1
1:A:47:LEU:HD23	1:A:47:LEU:O	0.48	2.09	14	1
1:A:90:ARG:HH12	1:A:179:TYR:CB	0.48	2.22	14	1
1:A:61:ARG:NH2	1:A:64:ALA:HB3	0.48	2.24	15	1
1:A:177:LEU:HD13	1:A:177:LEU:O	0.47	2.09	14	1
1:A:161:VAL:O	1:A:162:LYS:C	0.47	2.56	6	6
1:A:69:LEU:HD23	1:A:69:LEU:C	0.47	2.34	3	1
1:A:80:LEU:HD23	1:A:80:LEU:C	0.47	2.33	6	1
1:A:145:GLY:O	1:A:149:THR:CG2	0.47	2.62	9	1
1:A:48:ILE:C	1:A:61:ARG:HH21	0.47	2.18	11	1
1:A:46:MET:C	1:A:46:MET:SD	0.47	2.97	14	1
1:A:69:LEU:N	1:A:69:LEU:CD1	0.47	2.78	14	1
1:A:95:LEU:C	1:A:95:LEU:CD2	0.47	2.85	11	5
1:A:75:LEU:HD23	1:A:75:LEU:O	0.47	2.10	5	1
1:A:152:ALA:HB1	1:A:167:LEU:HD11	0.47	1.85	15	2
1:A:81:ASP:O	1:A:84:VAL:HG22	0.47	2.08	9	1
1:A:49:LEU:HD23	1:A:49:LEU:C	0.47	2.35	13	1
1:A:39:VAL:CG2	1:A:40:ALA:N	0.47	2.77	2	6
1:A:156:MET:CG	1:A:160:PHE:CD2	0.47	2.98	5	1
1:A:130:THR:O	1:A:131:LEU:O	0.47	2.31	6	2
1:A:67:PHE:N	1:A:67:PHE:CD1	0.47	2.81	15	1
1:A:119:ILE:CD1	1:A:174:ALA:HB3	0.47	2.39	15	1
1:A:42:LEU:HG	1:A:43:THR:N	0.47	2.25	1	6
1:A:17:VAL:CG2	1:A:162:LYS:O	0.47	2.62	4	2
1:A:69:LEU:HD13	1:A:113:PHE:CE1	0.47	2.44	9	1
1:A:127:ILE:O	1:A:127:ILE:HD13	0.47	2.08	12	1
1:A:153:VAL:O	1:A:156:MET:CG	0.47	2.63	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:PHE:CD1	1:A:87:PHE:C	0.47	2.92	2	6
1:A:144:LEU:HD23	1:A:144:LEU:O	0.47	2.10	2	3
1:A:137:LEU:N	1:A:137:LEU:CD2	0.47	2.77	4	1
1:A:49:LEU:CB	1:A:182:TYR:OH	0.47	2.63	6	1
1:A:45:SER:C	1:A:61:ARG:HE	0.47	2.17	12	1
1:A:166:GLN:H	1:A:166:GLN:CD	0.47	2.17	13	1
1:A:40:ALA:O	1:A:43:THR:OG1	0.47	2.32	6	4
1:A:49:LEU:HD12	1:A:49:LEU:O	0.47	2.10	5	1
1:A:134:GLU:O	1:A:135:ASN:O	0.47	2.33	11	1
1:A:116:LEU:N	1:A:117:PRO:CD	0.46	2.77	5	5
1:A:39:VAL:HG23	1:A:40:ALA:N	0.46	2.25	2	1
1:A:90:ARG:NH2	1:A:94:GLY:CA	0.46	2.79	14	2
1:A:80:LEU:HD13	1:A:80:LEU:N	0.46	2.15	8	1
1:A:73:LEU:C	1:A:73:LEU:CD1	0.46	2.87	10	1
1:A:66:LEU:HD13	1:A:66:LEU:O	0.46	2.11	12	3
1:A:134:GLU:O	1:A:135:ASN:CG	0.46	2.58	11	2
1:A:61:ARG:HH12	1:A:65:MET:CE	0.46	2.23	12	1
1:A:156:MET:CG	1:A:157:GLY:N	0.46	2.79	1	4
1:A:73:LEU:O	1:A:73:LEU:HD23	0.46	2.10	8	1
1:A:78:ASP:O	1:A:78:ASP:OD1	0.46	2.34	3	2
1:A:65:MET:O	1:A:68:LEU:CB	0.46	2.63	2	1
1:A:65:MET:O	1:A:68:LEU:CD1	0.46	2.64	7	1
1:A:70:ILE:HG23	1:A:71:PHE:N	0.46	2.24	11	2
1:A:132:LEU:N	1:A:132:LEU:HD23	0.46	2.25	10	1
1:A:58:GLY:O	1:A:61:ARG:NH1	0.46	2.43	14	1
1:A:70:ILE:N	1:A:70:ILE:CD1	0.46	2.78	14	1
1:A:159:LYS:O	1:A:160:PHE:O	0.46	2.34	3	7
1:A:87:PHE:CD2	1:A:115:TRP:CZ2	0.46	3.03	4	1
1:A:163:ALA:O	1:A:164:ASN:O	0.46	2.34	15	4
1:A:132:LEU:H	1:A:132:LEU:HD13	0.46	1.70	6	1
1:A:65:MET:HE2	1:A:114:LEU:HD11	0.46	1.87	9	1
1:A:70:ILE:CG2	1:A:71:PHE:N	0.46	2.77	7	6
1:A:115:TRP:CZ3	1:A:175:ILE:HG23	0.46	2.46	4	1
1:A:61:ARG:HH22	1:A:114:LEU:CD1	0.46	2.24	12	1
1:A:170:LYS:HB2	1:A:170:LYS:HZ3	0.46	1.71	14	1
1:A:75:LEU:O	1:A:78:ASP:OD1	0.46	2.34	3	1
1:A:90:ARG:CB	1:A:115:TRP:CH2	0.46	2.98	10	2
1:A:141:SER:OG	1:A:177:LEU:HD13	0.46	2.10	10	1
1:A:70:ILE:CG1	1:A:71:PHE:N	0.46	2.78	13	1
1:A:150:ILE:CG2	1:A:151:ALA:N	0.45	2.78	3	3
1:A:110:LEU:HD23	1:A:110:LEU:N	0.45	2.26	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:LEU:HD13	1:A:178:LEU:N	0.45	2.26	11	1
1:A:37:LEU:HD13	1:A:37:LEU:O	0.45	2.11	1	1
1:A:79:GLU:O	1:A:80:LEU:O	0.45	2.34	10	3
1:A:80:LEU:HD23	1:A:80:LEU:H	0.45	1.71	7	1
1:A:114:LEU:HD22	1:A:114:LEU:N	0.45	2.27	9	1
1:A:115:TRP:CE3	1:A:175:ILE:HG23	0.45	2.46	13	1
1:A:14:SER:OG	1:A:156:MET:O	0.45	2.32	9	3
1:A:142:TYR:CD1	1:A:177:LEU:HD13	0.45	2.47	3	1
1:A:68:LEU:HD12	1:A:113:PHE:CE1	0.45	2.46	11	1
1:A:120:LEU:O	1:A:120:LEU:HD13	0.45	2.11	12	1
1:A:44:ILE:HG23	1:A:45:SER:N	0.45	2.26	14	3
1:A:11:SER:OG	1:A:156:MET:CE	0.45	2.65	3	1
1:A:122:PHE:CE1	1:A:177:LEU:CD1	0.45	3.00	3	1
1:A:131:LEU:HD12	1:A:131:LEU:H	0.45	1.70	5	1
1:A:132:LEU:H	1:A:132:LEU:HD23	0.45	1.69	10	1
1:A:164:ASN:HD22	1:A:166:GLN:N	0.45	2.09	12	1
1:A:158:GLU:O	1:A:159:LYS:O	0.45	2.34	7	3
1:A:67:PHE:CD1	1:A:68:LEU:N	0.45	2.84	8	1
1:A:125:ILE:CG2	1:A:142:TYR:CE1	0.45	3.00	10	1
1:A:128:SER:O	1:A:131:LEU:O	0.45	2.35	2	1
1:A:68:LEU:HD13	1:A:117:PRO:HG2	0.45	1.87	5	1
1:A:30:GLY:O	1:A:34:ASP:OD1	0.45	2.35	6	1
1:A:152:ALA:CB	1:A:167:LEU:HD22	0.45	2.41	5	1
1:A:75:LEU:O	1:A:78:ASP:O	0.45	2.35	10	4
1:A:90:ARG:HB3	1:A:115:TRP:CH2	0.45	2.47	10	1
1:A:31:ARG:O	1:A:34:ASP:CG	0.45	2.60	2	3
1:A:142:TYR:OH	1:A:181:ALA:CB	0.45	2.65	12	2
1:A:167:LEU:O	1:A:170:LYS:CG	0.45	2.65	7	3
1:A:90:ARG:HH11	1:A:115:TRP:NE1	0.45	2.10	6	1
1:A:49:LEU:C	1:A:49:LEU:CD1	0.45	2.90	7	1
1:A:160:PHE:O	1:A:161:VAL:CG1	0.45	2.65	12	1
1:A:38:ILE:HD11	1:A:71:PHE:CE2	0.45	2.47	3	1
1:A:79:GLU:N	1:A:79:GLU:CD	0.45	2.75	11	1
1:A:144:LEU:HD13	1:A:144:LEU:O	0.45	2.12	6	1
1:A:116:LEU:HD12	1:A:116:LEU:N	0.45	2.26	9	1
1:A:14:SER:O	1:A:15:PRO:O	0.44	2.35	4	2
1:A:86:ILE:O	1:A:89:SER:OG	0.44	2.34	8	1
1:A:71:PHE:O	1:A:74:ILE:HG22	0.44	2.12	5	3
1:A:82:GLU:O	1:A:83:LYS:C	0.44	2.61	1	1
1:A:95:LEU:CD1	1:A:96:SER:N	0.44	2.73	2	1
1:A:135:ASN:O	1:A:135:ASN:OD1	0.44	2.34	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:LEU:O	1:A:46:MET:CG	0.44	2.65	3	1
1:A:118:ALA:CB	1:A:178:LEU:CD1	0.44	2.95	3	1
1:A:155:LYS:O	1:A:159:LYS:O	0.44	2.35	3	1
1:A:164:ASN:CG	1:A:165:PHE:H	0.44	2.19	3	1
1:A:133:SER:O	1:A:134:GLU:CD	0.44	2.60	2	2
1:A:78:ASP:O	1:A:79:GLU:O	0.44	2.35	11	2
1:A:149:THR:HG21	1:A:170:LYS:HE3	0.44	1.87	8	1
1:A:61:ARG:O	1:A:61:ARG:NE	0.44	2.51	15	1
1:A:31:ARG:O	1:A:34:ASP:OD2	0.44	2.36	6	3
1:A:46:MET:C	1:A:182:TYR:OH	0.44	2.61	7	1
1:A:115:TRP:CD1	1:A:115:TRP:C	0.44	2.95	8	2
1:A:177:LEU:C	1:A:177:LEU:CD2	0.44	2.84	11	1
1:A:38:ILE:O	1:A:41:GLY:N	0.44	2.51	13	1
1:A:148:VAL:HG22	1:A:170:LYS:HD2	0.44	1.89	14	1
1:A:39:VAL:HG22	1:A:117:PRO:O	0.44	2.12	15	1
1:A:80:LEU:O	1:A:81:ASP:CG	0.44	2.61	13	3
1:A:74:ILE:CG2	1:A:75:LEU:N	0.44	2.81	10	2
1:A:132:LEU:C	1:A:132:LEU:CD1	0.44	2.91	7	1
1:A:81:ASP:CG	1:A:82:GLU:H	0.44	2.21	11	1
1:A:39:VAL:CG2	1:A:117:PRO:O	0.44	2.66	15	1
1:A:81:ASP:CG	1:A:82:GLU:N	0.44	2.75	2	1
1:A:134:GLU:O	1:A:135:ASN:C	0.44	2.61	2	1
1:A:132:LEU:CD1	1:A:132:LEU:N	0.44	2.78	6	1
1:A:158:GLU:O	1:A:159:LYS:C	0.44	2.60	7	1
1:A:132:LEU:O	1:A:133:SER:O	0.44	2.36	10	2
1:A:107:PHE:CD1	1:A:107:PHE:C	0.44	2.94	2	1
1:A:80:LEU:C	1:A:81:ASP:CG	0.44	2.86	10	1
1:A:109:MET:SD	1:A:113:PHE:CE2	0.44	3.11	12	1
1:A:73:LEU:C	1:A:73:LEU:HD23	0.44	2.38	14	1
1:A:75:LEU:O	1:A:78:ASP:CG	0.44	2.60	5	4
1:A:46:MET:O	1:A:182:TYR:OH	0.44	2.33	2	3
1:A:115:TRP:CD1	1:A:175:ILE:CG2	0.44	3.00	7	1
1:A:132:LEU:CD2	1:A:133:SER:H	0.44	2.25	14	1
1:A:133:SER:O	1:A:134:GLU:C	0.44	2.61	15	1
1:A:166:GLN:CD	1:A:166:GLN:C	0.44	2.86	4	1
1:A:48:ILE:HD12	1:A:61:ARG:NH1	0.44	2.28	9	1
1:A:126:ALA:HB2	1:A:142:TYR:CE1	0.44	2.48	11	1
1:A:135:ASN:C	1:A:135:ASN:OD1	0.44	2.61	11	1
1:A:116:LEU:C	1:A:116:LEU:CD1	0.44	2.91	15	1
1:A:131:LEU:O	1:A:132:LEU:O	0.43	2.36	5	2
1:A:183:PHE:CD2	1:A:184:ALA:O	0.43	2.71	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ILE:CG2	1:A:61:ARG:NH2	0.43	2.81	11	1
1:A:129:GLN:O	1:A:132:LEU:O	0.43	2.36	14	1
1:A:125:ILE:HD13	1:A:125:ILE:C	0.43	2.36	1	1
1:A:45:SER:O	1:A:61:ARG:NH1	0.43	2.49	6	1
1:A:69:LEU:HD13	1:A:113:PHE:CG	0.43	2.48	7	1
1:A:155:LYS:O	1:A:158:GLU:O	0.43	2.36	7	1
1:A:83:LYS:NZ	1:A:168:ILE:HD13	0.43	2.28	15	1
1:A:83:LYS:O	1:A:87:PHE:N	0.43	2.48	1	2
1:A:62:VAL:O	1:A:65:MET:CG	0.43	2.67	6	1
1:A:132:LEU:CD2	1:A:132:LEU:N	0.43	2.80	10	1
1:A:96:SER:O	1:A:97:TRP:O	0.43	2.37	5	3
1:A:79:GLU:CD	1:A:79:GLU:C	0.43	2.87	7	3
1:A:90:ARG:NH2	1:A:179:TYR:CB	0.43	2.82	6	1
1:A:16:ALA:O	1:A:17:VAL:C	0.43	2.61	10	1
1:A:164:ASN:OD1	1:A:166:GLN:N	0.43	2.51	11	1
1:A:69:LEU:C	1:A:69:LEU:CD2	0.43	2.88	12	1
1:A:17:VAL:O	1:A:17:VAL:HG12	0.43	2.14	14	1
1:A:132:LEU:O	1:A:133:SER:C	0.43	2.61	1	1
1:A:183:PHE:CD1	1:A:183:PHE:C	0.43	2.97	14	1
1:A:76:LEU:O	1:A:78:ASP:OD2	0.43	2.37	15	1
1:A:106:PHE:O	1:A:107:PHE:C	0.43	2.61	10	3
1:A:82:GLU:CD	1:A:82:GLU:C	0.43	2.86	4	2
1:A:148:VAL:CG2	1:A:149:THR:N	0.43	2.81	2	1
1:A:122:PHE:CE1	1:A:142:TYR:OH	0.43	2.69	4	1
1:A:131:LEU:C	1:A:131:LEU:CD1	0.43	2.92	13	2
1:A:152:ALA:HB1	1:A:167:LEU:HD21	0.43	1.90	4	1
1:A:33:LEU:CD2	1:A:33:LEU:H	0.43	2.26	14	1
1:A:44:ILE:CG2	1:A:45:SER:N	0.43	2.82	14	4
1:A:125:ILE:O	1:A:128:SER:OG	0.43	2.36	4	1
1:A:65:MET:SD	1:A:110:LEU:O	0.43	2.77	5	1
1:A:78:ASP:OD2	1:A:79:GLU:OE2	0.43	2.37	7	1
1:A:134:GLU:OE2	1:A:134:GLU:O	0.43	2.37	10	1
1:A:167:LEU:HD13	1:A:167:LEU:C	0.43	2.38	14	1
1:A:166:GLN:OE1	1:A:166:GLN:O	0.43	2.36	15	1
1:A:78:ASP:O	1:A:78:ASP:CG	0.43	2.61	3	1
1:A:111:LEU:C	1:A:111:LEU:CD1	0.43	2.91	3	1
1:A:92:THR:CG2	1:A:93:SER:N	0.43	2.82	4	2
1:A:134:GLU:CD	1:A:134:GLU:C	0.43	2.87	14	2
1:A:49:LEU:C	1:A:51:TYR:H	0.43	2.22	2	1
1:A:90:ARG:HH21	1:A:94:GLY:N	0.43	2.12	2	1
1:A:134:GLU:O	1:A:135:ASN:OD1	0.43	2.37	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:TYR:CD1	1:A:142:TYR:N	0.43	2.85	3	2
1:A:128:SER:O	1:A:133:SER:OG	0.43	2.37	6	1
1:A:73:LEU:HD12	1:A:73:LEU:O	0.43	2.14	10	1
1:A:62:VAL:HG13	1:A:63:VAL:N	0.43	2.29	15	1
1:A:62:VAL:CG2	1:A:63:VAL:N	0.43	2.82	8	2
1:A:90:ARG:CZ	1:A:115:TRP:HE1	0.43	2.26	5	1
1:A:69:LEU:HD23	1:A:113:PHE:CE2	0.43	2.48	11	2
1:A:170:LYS:NZ	1:A:170:LYS:CB	0.43	2.82	14	1
1:A:49:LEU:CD1	1:A:182:TYR:OH	0.42	2.67	6	1
1:A:80:LEU:O	1:A:81:ASP:OD1	0.42	2.37	7	1
1:A:135:ASN:HD22	1:A:135:ASN:C	0.42	2.22	1	1
1:A:114:LEU:HD23	1:A:114:LEU:C	0.42	2.39	2	1
1:A:157:GLY:C	1:A:158:GLU:CD	0.42	2.86	7	2
1:A:8:GLY:CA	1:A:120:LEU:HD23	0.42	2.44	4	1
1:A:92:THR:O	1:A:95:LEU:HD23	0.42	2.15	6	2
1:A:135:ASN:OD1	1:A:135:ASN:C	0.42	2.61	7	1
1:A:158:GLU:CD	1:A:158:GLU:C	0.42	2.86	8	1
1:A:39:VAL:CB	1:A:117:PRO:O	0.42	2.68	9	1
1:A:69:LEU:CD1	1:A:113:PHE:CZ	0.42	3.02	13	1
1:A:9:ILE:HD13	1:A:36:PHE:CE2	0.42	2.49	6	1
1:A:165:PHE:O	1:A:168:ILE:CG1	0.42	2.67	9	2
1:A:136:PRO:O	1:A:140:LEU:HD13	0.42	2.13	13	1
1:A:149:THR:CG2	1:A:150:ILE:N	0.42	2.82	14	1
1:A:66:LEU:HD21	1:A:110:LEU:HD11	0.42	1.90	7	1
1:A:176:VAL:HG23	1:A:177:LEU:N	0.42	2.29	7	1
1:A:110:LEU:N	1:A:110:LEU:CD1	0.42	2.83	10	1
1:A:72:ALA:HB2	1:A:113:PHE:CZ	0.42	2.49	11	1
1:A:45:SER:O	1:A:48:ILE:HG22	0.42	2.14	15	1
1:A:87:PHE:O	1:A:115:TRP:CH2	0.42	2.73	15	1
1:A:13:PHE:O	1:A:14:SER:C	0.42	2.62	1	1
1:A:79:GLU:OE2	1:A:80:LEU:O	0.42	2.37	4	1
1:A:36:PHE:CD1	1:A:36:PHE:C	0.42	2.95	7	1
1:A:177:LEU:C	1:A:177:LEU:HD12	0.42	2.39	8	1
1:A:148:VAL:HG13	1:A:149:THR:N	0.42	2.30	9	1
1:A:76:LEU:HD11	1:A:87:PHE:CE1	0.42	2.49	3	1
1:A:3:MET:O	1:A:7:LEU:CD2	0.42	2.67	14	1
1:A:165:PHE:O	1:A:168:ILE:HG13	0.42	2.15	15	1
1:A:122:PHE:CZ	1:A:142:TYR:CE2	0.42	3.08	2	1
1:A:129:GLN:OE1	1:A:138:VAL:HG21	0.42	2.15	3	1
1:A:14:SER:CB	1:A:156:MET:SD	0.42	3.08	5	1
1:A:165:PHE:CG	1:A:166:GLN:N	0.42	2.88	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ARG:HD2	1:A:61:ARG:H	0.42	1.75	9	1
1:A:159:LYS:CB	1:A:159:LYS:NZ	0.42	2.82	10	1
1:A:159:LYS:C	1:A:160:PHE:O	0.42	2.63	15	2
1:A:65:MET:CB	1:A:113:PHE:CE1	0.42	3.02	2	1
1:A:131:LEU:HD12	1:A:131:LEU:C	0.42	2.40	2	1
1:A:16:ALA:C	1:A:17:VAL:O	0.42	2.61	13	4
1:A:76:LEU:O	1:A:78:ASP:OD1	0.42	2.38	5	1
1:A:170:LYS:HG3	1:A:171:VAL:N	0.42	2.29	8	1
1:A:78:ASP:OD1	1:A:78:ASP:C	0.42	2.62	10	1
1:A:83:LYS:HZ1	1:A:168:ILE:CD1	0.42	2.28	10	1
1:A:96:SER:O	1:A:97:TRP:C	0.42	2.63	2	1
1:A:59:PHE:O	1:A:63:VAL:HG23	0.42	2.15	6	1
1:A:140:LEU:HD13	1:A:140:LEU:O	0.42	2.15	8	1
1:A:115:TRP:CG	1:A:116:LEU:N	0.42	2.87	10	1
1:A:95:LEU:HD22	1:A:96:SER:CA	0.41	2.45	1	2
1:A:81:ASP:O	1:A:82:GLU:C	0.41	2.63	4	1
1:A:111:LEU:HD13	1:A:179:TYR:CZ	0.41	2.50	6	1
1:A:80:LEU:O	1:A:80:LEU:HD22	0.41	2.14	8	1
1:A:37:LEU:HD22	1:A:37:LEU:C	0.41	2.40	14	1
1:A:74:ILE:O	1:A:77:SER:OG	0.41	2.35	5	1
1:A:150:ILE:O	1:A:151:ALA:C	0.41	2.62	2	1
1:A:74:ILE:CD1	1:A:75:LEU:N	0.41	2.77	7	1
1:A:161:VAL:CG2	1:A:164:ASN:OD1	0.41	2.69	7	1
1:A:161:VAL:CG1	1:A:164:ASN:OD1	0.41	2.69	7	1
1:A:166:GLN:HE22	1:A:169:ARG:NH1	0.41	2.14	2	1
1:A:82:GLU:C	1:A:82:GLU:OE1	0.41	2.64	4	1
1:A:169:ARG:CD	1:A:169:ARG:C	0.41	2.93	5	1
1:A:135:ASN:O	1:A:139:MET:CG	0.41	2.69	7	2
1:A:131:LEU:C	1:A:131:LEU:HD13	0.41	2.40	13	1
1:A:62:VAL:O	1:A:110:LEU:HD12	0.41	2.15	1	1
1:A:59:PHE:CE2	1:A:63:VAL:HG21	0.41	2.50	3	1
1:A:166:GLN:CD	1:A:166:GLN:O	0.41	2.63	4	1
1:A:134:GLU:C	1:A:135:ASN:CG	0.41	2.88	5	1
1:A:132:LEU:C	1:A:132:LEU:HD13	0.41	2.41	7	1
1:A:176:VAL:CG1	1:A:177:LEU:N	0.41	2.82	9	2
1:A:127:ILE:N	1:A:127:ILE:CD1	0.41	2.83	13	1
1:A:81:ASP:HB3	1:A:84:VAL:HG13	0.41	1.92	15	1
1:A:127:ILE:HD13	1:A:127:ILE:C	0.41	2.40	3	1
1:A:111:LEU:O	1:A:111:LEU:HD12	0.41	2.15	4	1
1:A:87:PHE:CE2	1:A:116:LEU:HD12	0.41	2.51	14	1
1:A:62:VAL:CG1	1:A:63:VAL:N	0.41	2.83	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:LEU:HD12	1:A:178:LEU:H	0.41	1.73	2	1
1:A:49:LEU:HD23	1:A:182:TYR:CE1	0.41	2.50	5	1
1:A:5:PHE:CE1	1:A:40:ALA:HB1	0.41	2.49	8	1
1:A:5:PHE:CE1	1:A:37:LEU:HD22	0.41	2.51	1	1
1:A:167:LEU:O	1:A:170:LYS:HG3	0.41	2.15	5	1
1:A:46:MET:HG3	1:A:182:TYR:CZ	0.41	2.51	12	1
1:A:29:ARG:O	1:A:31:ARG:N	0.41	2.53	14	1
1:A:138:VAL:O	1:A:142:TYR:CB	0.41	2.69	1	1
1:A:48:ILE:CG2	1:A:61:ARG:HE	0.41	2.29	3	1
1:A:70:ILE:HD13	1:A:70:ILE:C	0.41	2.41	3	1
1:A:81:ASP:O	1:A:82:GLU:CG	0.41	2.69	8	1
1:A:8:GLY:O	1:A:11:SER:OG	0.41	2.36	10	1
1:A:46:MET:SD	1:A:46:MET:O	0.41	2.79	11	1
1:A:165:PHE:CD1	1:A:165:PHE:O	0.41	2.74	11	1
1:A:122:PHE:CE1	1:A:177:LEU:HD13	0.41	2.51	2	1
1:A:122:PHE:CE2	1:A:177:LEU:HD11	0.41	2.51	8	1
1:A:65:MET:O	1:A:68:LEU:N	0.40	2.55	2	1
1:A:146:MET:O	1:A:150:ILE:HG22	0.40	2.15	7	1
1:A:158:GLU:O	1:A:159:LYS:CG	0.40	2.69	10	1
1:A:115:TRP:CE3	1:A:175:ILE:CG2	0.40	3.05	13	1
1:A:159:LYS:O	1:A:160:PHE:CB	0.40	2.68	2	1
1:A:65:MET:SD	1:A:110:LEU:C	0.40	3.05	5	1
1:A:83:LYS:O	1:A:86:ILE:CG1	0.40	2.69	5	1
1:A:50:GLY:O	1:A:51:TYR:CD2	0.40	2.74	11	1
1:A:59:PHE:CZ	1:A:63:VAL:HG21	0.40	2.52	13	1
1:A:133:SER:O	1:A:134:GLU:OE2	0.40	2.40	1	1
1:A:69:LEU:CD1	1:A:113:PHE:CD1	0.40	3.05	7	1
1:A:122:PHE:O	1:A:125:ILE:CG2	0.40	2.70	12	1
1:A:119:ILE:HD11	1:A:174:ALA:HB3	0.40	1.92	14	1
1:A:146:MET:CG	1:A:147:ALA:N	0.40	2.84	15	1
1:A:122:PHE:CE1	1:A:177:LEU:HD11	0.40	2.52	3	1
1:A:107:PHE:CG	1:A:108:GLY:N	0.40	2.89	6	1
1:A:149:THR:HG21	1:A:170:LYS:CB	0.40	2.47	6	1
1:A:112:ALA:HA	1:A:115:TRP:CZ3	0.40	2.50	7	1
1:A:129:GLN:O	1:A:133:SER:O	0.40	2.40	7	1
1:A:139:MET:CG	1:A:140:LEU:N	0.40	2.84	8	1
1:A:177:LEU:HD13	1:A:178:LEU:H	0.40	1.76	11	1
1:A:90:ARG:NH2	1:A:180:LEU:HD23	0.40	2.31	12	1
1:A:142:TYR:O	1:A:146:MET:CB	0.40	2.69	13	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/208 (76%)	131±3 (83±2%)	13±3 (8±2%)	15±1 (9±1%)	1	11
All	All	2370/3120 (76%)	1960 (83%)	189 (8%)	221 (9%)	1	11

All 36 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	163	ALA	15
1	A	118	ALA	14
1	A	119	ILE	13
1	A	95	LEU	13
1	A	160	PHE	12
1	A	184	ALA	12
1	A	78	ASP	11
1	A	17	VAL	10
1	A	157	GLY	8
1	A	164	ASN	8
1	A	29	ARG	7
1	A	16	ALA	6
1	A	50	GLY	6
1	A	133	SER	6
1	A	97	TRP	6
1	A	13	PHE	6
1	A	15	PRO	5
1	A	159	LYS	5
1	A	79	GLU	5
1	A	30	GLY	5
1	A	132	LEU	5
1	A	136	PRO	5
1	A	80	LEU	4
1	A	82	GLU	4
1	A	162	LYS	4
1	A	106	PHE	4
1	A	3	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	161	VAL	4
1	A	96	SER	3
1	A	83	LYS	2
1	A	51	TYR	2
1	A	131	LEU	2
1	A	135	ASN	2
1	A	107	PHE	1
1	A	134	GLU	1
1	A	57	PHE	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/171 (74%)	98±5 (78±4%)	28±5 (22±4%)	2	29
All	All	1890/2565 (74%)	1468 (78%)	422 (22%)	2	29

All 102 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	42	LEU	15
1	A	95	LEU	13
1	A	170	LYS	13
1	A	125	ILE	12
1	A	90	ARG	12
1	A	138	VAL	9
1	A	182	TYR	9
1	A	160	PHE	9
1	A	63	VAL	8
1	A	119	ILE	8
1	A	68	LEU	8
1	A	87	PHE	8
1	A	45	SER	8
1	A	168	ILE	7
1	A	175	ILE	7
1	A	129	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	83	LYS	7
1	A	65	MET	6
1	A	82	GLU	6
1	A	110	LEU	6
1	A	62	VAL	6
1	A	114	LEU	6
1	A	177	LEU	6
1	A	69	LEU	5
1	A	73	LEU	5
1	A	84	VAL	5
1	A	131	LEU	5
1	A	171	VAL	5
1	A	111	LEU	5
1	A	127	ILE	5
1	A	36	PHE	5
1	A	49	LEU	5
1	A	81	ASP	5
1	A	92	THR	5
1	A	120	LEU	5
1	A	132	LEU	5
1	A	76	LEU	5
1	A	37	LEU	4
1	A	38	ILE	4
1	A	70	ILE	4
1	A	75	LEU	4
1	A	172	THR	4
1	A	116	LEU	4
1	A	66	LEU	4
1	A	109	MET	4
1	A	5	PHE	4
1	A	47	LEU	4
1	A	80	LEU	4
1	A	61	ARG	4
1	A	178	LEU	4
1	A	7	LEU	3
1	A	17	VAL	3
1	A	79	GLU	3
1	A	130	THR	3
1	A	167	LEU	3
1	A	48	ILE	3
1	A	162	LYS	3
1	A	165	PHE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	10	LEU	3
1	A	14	SER	3
1	A	46	MET	3
1	A	33	LEU	3
1	A	140	LEU	3
1	A	169	ARG	3
1	A	153	VAL	3
1	A	11	SER	3
1	A	156	MET	3
1	A	9	ILE	3
1	A	91	MET	2
1	A	135	ASN	2
1	A	150	ILE	2
1	A	71	PHE	2
1	A	180	LEU	2
1	A	164	ASN	2
1	A	166	GLN	2
1	A	39	VAL	2
1	A	74	ILE	2
1	A	57	PHE	2
1	A	59	PHE	2
1	A	146	MET	2
1	A	154	PHE	2
1	A	183	PHE	2
1	A	3	MET	2
1	A	149	THR	2
1	A	67	PHE	1
1	A	113	PHE	1
1	A	107	PHE	1
1	A	115	TRP	1
1	A	161	VAL	1
1	A	155	LYS	1
1	A	34	ASP	1
1	A	133	SER	1
1	A	144	LEU	1
1	A	44	ILE	1
1	A	137	LEU	1
1	A	29	ARG	1
1	A	158	GLU	1
1	A	159	LYS	1
1	A	134	GLU	1
1	A	139	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	93	SER	1
1	A	176	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 30% for the well-defined parts and 28% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_CcdA_reduced*

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	765
Number of shifts mapped to atoms	765
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	163	-0.61 ± 0.15	Should be checked
$^{13}\text{C}_\beta$	131	0.40 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	157	-0.53 ± 0.12	Should be applied
^{15}N	156	0.45 ± 0.22	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 30%, i.e. 676 atoms were assigned a chemical shift out of a possible 2247. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	559/794 (70%)	140/324 (43%)	281/316 (89%)	138/154 (90%)
Sidechain	117/1223 (10%)	0/827 (0%)	117/372 (31%)	0/24 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/230 (0%)	0/113 (0%)	0/115 (0%)	0/2 (0%)
Overall	676/2247 (30%)	140/1264 (11%)	398/803 (50%)	138/180 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 28%, i.e. 765 atoms were assigned a chemical shift out of a possible 2733. 0 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	634/959 (66%)	158/390 (41%)	320/384 (83%)	156/185 (84%)
Sidechain	131/1514 (9%)	0/1023 (0%)	131/464 (28%)	0/27 (0%)
Aromatic	0/260 (0%)	0/128 (0%)	0/130 (0%)	0/2 (0%)
Overall	765/2733 (28%)	158/1541 (10%)	451/978 (46%)	156/214 (73%)

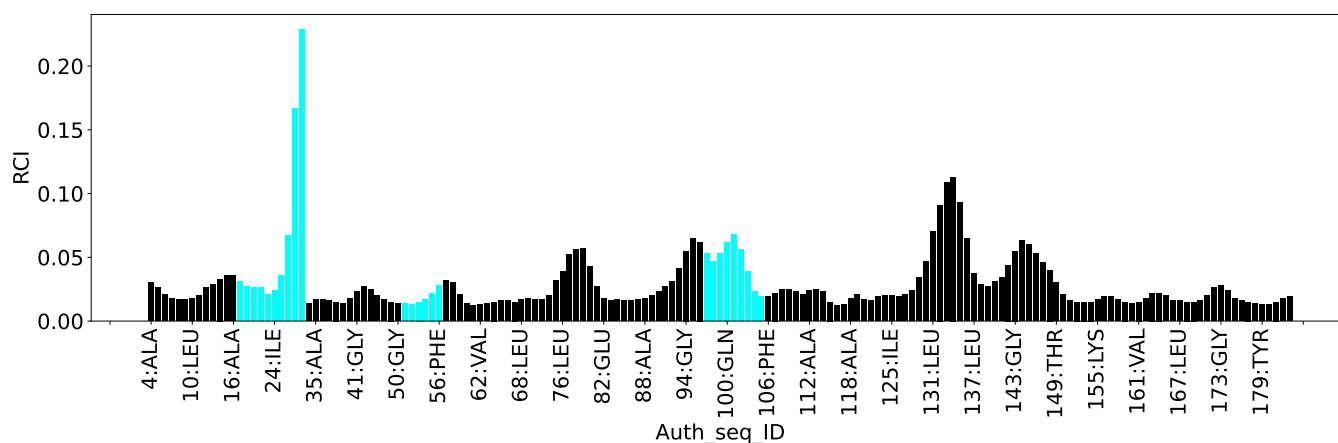
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



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	622
Intra-residue ($ i-j =0$)	125
Sequential ($ i-j =1$)	235
Medium range ($ i-j >1$ and $ i-j <5$)	161
Long range ($ i-j \geq 5$)	101
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	238
Number of unmapped restraints	0
Number of restraints per residue	4.1
Number of long range restraints per residue ¹	0.5

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	36.1	0.2
0.2-0.5 (Medium)	45.3	0.5
>0.5 (Large)	13.9	1.31

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)	4.2	1.57
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

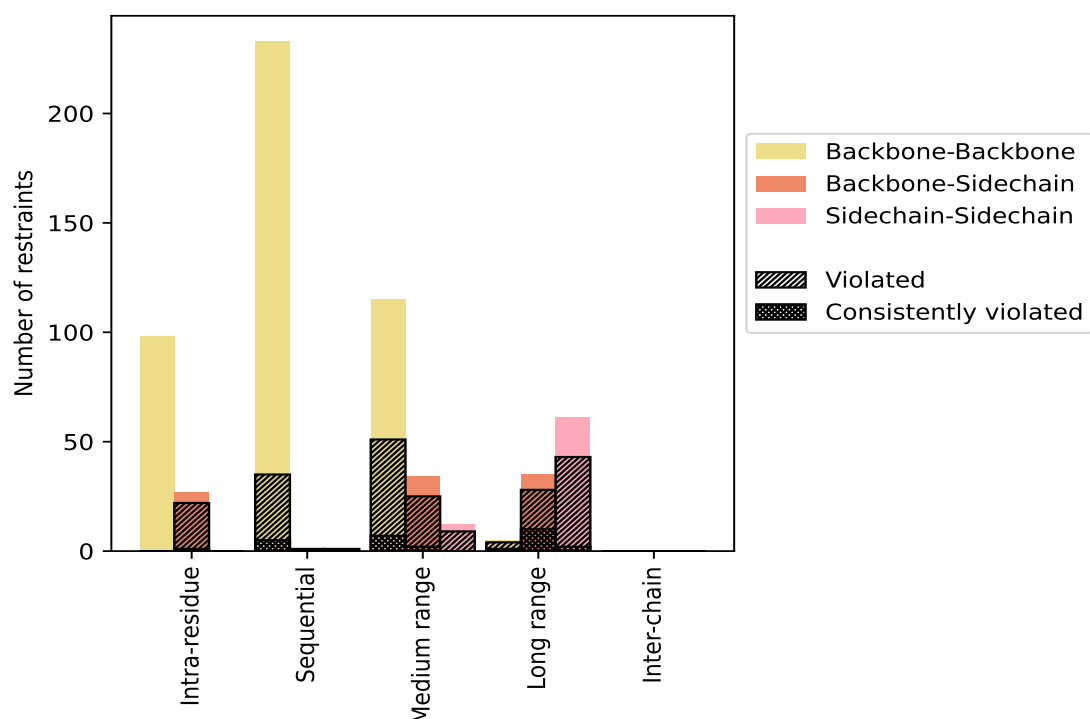
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	125	20.1	22	17.6	3.5	1	0.8	0.2
Backbone-Backbone	98	15.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	27	4.3	22	81.5	3.5	1	3.7	0.2
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	235	37.8	37	15.7	5.9	5	2.1	0.8
Backbone-Backbone	233	37.5	35	15.0	5.6	5	2.1	0.8
Backbone-Sidechain	1	0.2	1	100.0	0.2	0	0.0	0.0
Sidechain-Sidechain	1	0.2	1	100.0	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	161	25.9	85	52.8	13.7	9	5.6	1.4
Backbone-Backbone	115	18.5	51	44.3	8.2	7	6.1	1.1
Backbone-Sidechain	34	5.5	25	73.5	4.0	2	5.9	0.3
Sidechain-Sidechain	12	1.9	9	75.0	1.4	0	0.0	0.0
Long range ($i-j \geq 5$)	101	16.2	75	74.3	12.1	13	12.9	2.1
Backbone-Backbone	5	0.8	4	80.0	0.6	1	20.0	0.2
Backbone-Sidechain	35	5.6	28	80.0	4.5	10	28.6	1.6
Sidechain-Sidechain	61	9.8	43	70.5	6.9	2	3.3	0.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	622	100.0	219	35.2	35.2	28	4.5	4.5
Backbone-Backbone	451	72.5	90	20.0	14.5	13	2.9	2.1
Backbone-Sidechain	97	15.6	76	78.4	12.2	13	13.4	2.1
Sidechain-Sidechain	74	11.9	53	71.6	8.5	2	2.7	0.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	5	16	36	36	0	93	0.29	1.16	0.21	0.22
2	7	14	45	35	0	101	0.3	1.28	0.2	0.24
3	7	16	39	36	0	98	0.3	0.93	0.19	0.24
4	11	12	37	38	0	98	0.31	1.2	0.19	0.25
5	10	12	34	35	0	91	0.32	1.07	0.2	0.27
6	7	14	38	34	0	93	0.3	1.07	0.19	0.28
7	7	14	41	36	0	98	0.29	1.09	0.19	0.24
8	8	11	44	39	0	102	0.29	1.07	0.21	0.22
9	8	12	41	32	0	93	0.31	1.3	0.21	0.25
10	10	15	41	36	0	102	0.31	1.31	0.2	0.27

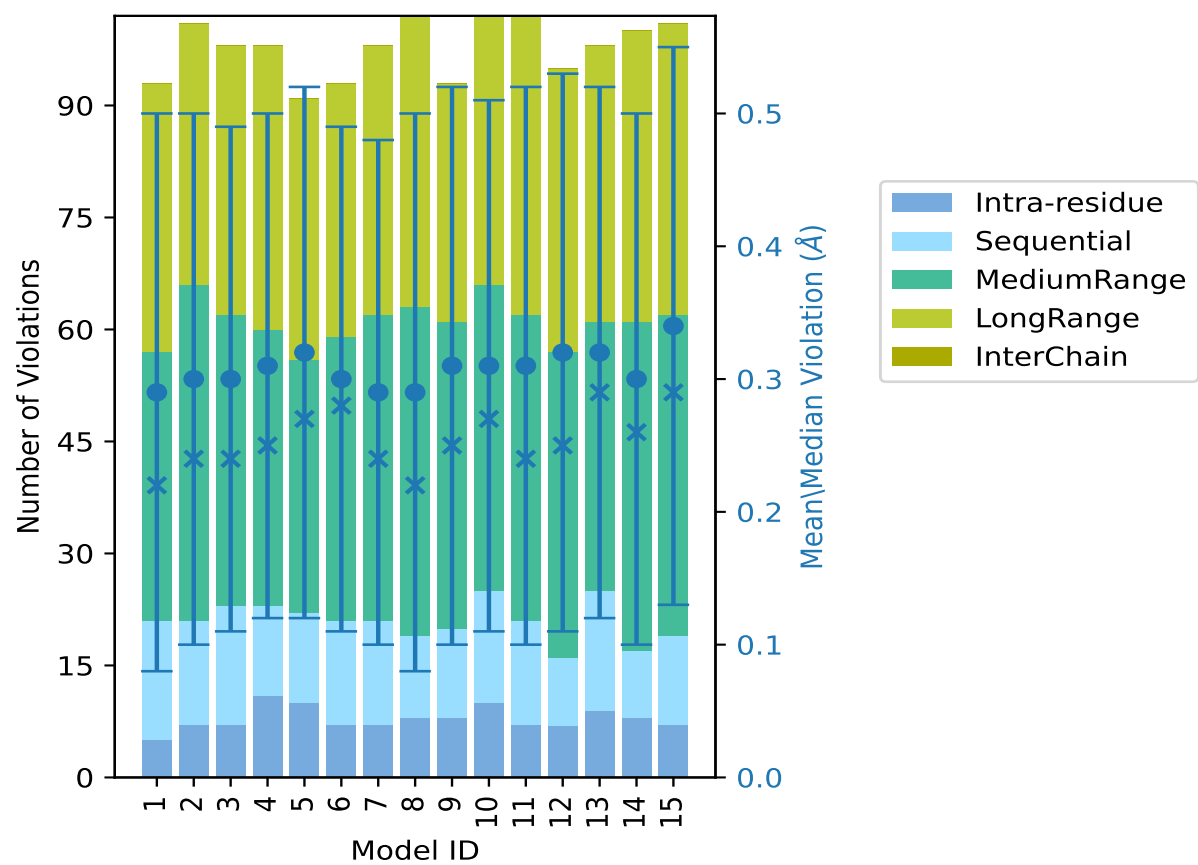
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	7	14	41	40	0	102	0.31	1.19	0.21	0.24
12	7	9	41	38	0	95	0.32	1.22	0.21	0.25
13	9	16	36	37	0	98	0.32	1.11	0.2	0.29
14	8	9	44	39	0	100	0.3	1.21	0.2	0.26
15	7	12	43	39	0	101	0.34	1.29	0.21	0.29

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

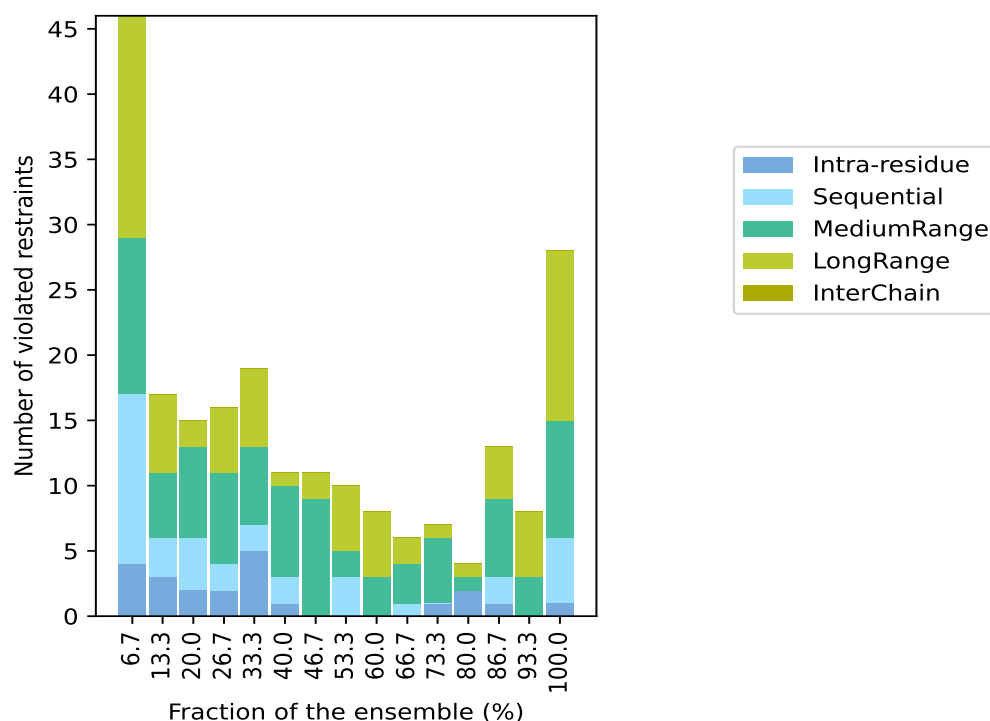
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 403(IR:103, SQ:198, MR:76, LR:26, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
4	13	12	17	0	46	1	6.7
3	3	5	6	0	17	2	13.3
2	4	7	2	0	15	3	20.0
2	2	7	5	0	16	4	26.7
5	2	6	6	0	19	5	33.3
1	2	7	1	0	11	6	40.0
0	0	9	2	0	11	7	46.7
0	3	2	5	0	10	8	53.3
0	0	3	5	0	8	9	60.0
0	1	3	2	0	6	10	66.7
1	0	5	1	0	7	11	73.3
2	0	1	1	0	4	12	80.0
1	2	6	4	0	13	13	86.7
0	0	3	5	0	8	14	93.3
1	5	9	13	0	28	15	100.0

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

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

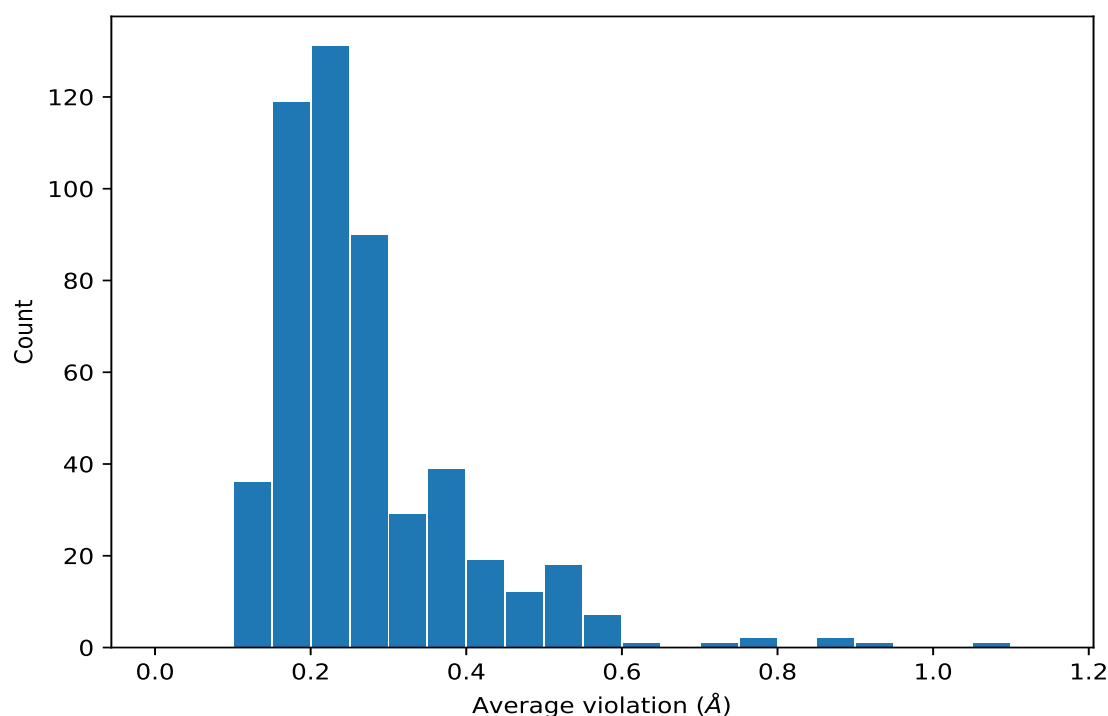
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	15	1.09	0.1	1.07
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	15	0.93	0.31	1.07
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	15	0.87	0.09	0.84
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	15	0.87	0.09	0.84
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	15	0.75	0.12	0.74
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	15	0.75	0.12	0.74
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	15	0.54	0.09	0.58
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	15	0.52	0.09	0.51
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	15	0.5	0.22	0.57
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	15	0.5	0.22	0.57
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	15	0.5	0.22	0.57
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	15	0.49	0.15	0.45
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	15	0.49	0.15	0.45
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	15	0.46	0.05	0.44
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	15	0.45	0.02	0.46
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	15	0.44	0.17	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	15	0.44	0.17	0.44
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	15	0.42	0.16	0.43
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	15	0.42	0.16	0.43
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	15	0.41	0.1	0.4
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	15	0.39	0.17	0.35
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	15	0.39	0.17	0.35
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	15	0.36	0.13	0.42
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	15	0.36	0.13	0.42
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	15	0.35	0.08	0.33
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	15	0.35	0.08	0.33
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	15	0.34	0.09	0.34
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	15	0.32	0.12	0.31
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	15	0.31	0.06	0.3
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	15	0.29	0.1	0.27
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	15	0.29	0.1	0.27
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	15	0.29	0.1	0.27
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	15	0.29	0.1	0.27
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	15	0.29	0.1	0.27
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	15	0.29	0.1	0.27
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	15	0.29	0.06	0.3
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	15	0.28	0.02	0.28
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	15	0.28	0.04	0.27
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	15	0.27	0.07	0.29
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	15	0.27	0.07	0.29
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	15	0.27	0.14	0.19
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	15	0.27	0.14	0.19
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	15	0.27	0.14	0.19
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	15	0.27	0.14	0.19
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	15	0.27	0.14	0.19
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	15	0.27	0.14	0.19
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	15	0.25	0.08	0.24
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	15	0.25	0.08	0.24
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	15	0.25	0.08	0.24
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	15	0.25	0.08	0.24
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	15	0.25	0.08	0.24
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	15	0.25	0.08	0.24
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	15	0.25	0.08	0.23
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	15	0.22	0.1	0.18
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	15	0.22	0.1	0.18
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	15	0.22	0.1	0.18
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	14	0.55	0.17	0.62
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	14	0.55	0.17	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	14	0.55	0.17	0.62
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	14	0.55	0.17	0.62
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	14	0.55	0.17	0.62
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	14	0.55	0.17	0.62
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	14	0.47	0.2	0.47
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	14	0.47	0.2	0.47
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	14	0.33	0.1	0.3
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	14	0.33	0.1	0.3
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	14	0.33	0.1	0.3
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	14	0.33	0.1	0.3
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	14	0.33	0.1	0.3
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	14	0.33	0.1	0.3
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	14	0.32	0.14	0.31
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	14	0.32	0.14	0.31
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	14	0.32	0.14	0.31
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	14	0.25	0.1	0.24
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	14	0.25	0.1	0.24
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	14	0.25	0.1	0.24
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	14	0.24	0.06	0.24
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	14	0.24	0.06	0.24
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	14	0.24	0.06	0.24
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	14	0.22	0.04	0.22
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	14	0.22	0.04	0.22
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	14	0.18	0.04	0.18
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	13	0.44	0.19	0.44
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	13	0.44	0.19	0.44
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	13	0.4	0.13	0.4
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	13	0.31	0.01	0.31
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	13	0.3	0.08	0.3
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	13	0.3	0.1	0.31
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	13	0.3	0.1	0.31
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	13	0.3	0.1	0.31
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	13	0.29	0.09	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	13	0.29	0.09	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	13	0.29	0.09	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	13	0.29	0.09	0.28
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	13	0.29	0.09	0.28
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	13	0.29	0.09	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	13	0.29	0.09	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	13	0.29	0.09	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	13	0.29	0.09	0.28
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	13	0.28	0.05	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	13	0.28	0.05	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	13	0.28	0.05	0.31
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	13	0.26	0.08	0.25
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	13	0.25	0.11	0.24
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	13	0.21	0.08	0.17
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	13	0.19	0.04	0.18
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	13	0.19	0.09	0.12
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	13	0.19	0.09	0.12
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	13	0.19	0.09	0.12
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	13	0.19	0.09	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	13	0.19	0.09	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	13	0.19	0.09	0.12
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	12	0.72	0.05	0.74
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	12	0.55	0.11	0.58
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	12	0.39	0.15	0.39
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	12	0.39	0.15	0.39
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	12	0.17	0.05	0.15
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	11	0.42	0.09	0.4
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	11	0.26	0.14	0.23
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	11	0.26	0.14	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	11	0.26	0.14	0.23
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	11	0.19	0.08	0.17
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	11	0.18	0.05	0.18
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	11	0.17	0.05	0.16
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	11	0.17	0.07	0.15
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	11	0.17	0.07	0.15
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	11	0.17	0.07	0.15
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	11	0.17	0.07	0.15
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	11	0.17	0.07	0.15
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	11	0.17	0.07	0.15
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	11	0.15	0.03	0.16
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	10	0.23	0.1	0.21
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	10	0.23	0.1	0.21
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	10	0.22	0.07	0.22
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	10	0.22	0.07	0.22
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	10	0.22	0.07	0.22
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	10	0.22	0.08	0.22
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	10	0.22	0.13	0.15
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	10	0.22	0.13	0.15
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	10	0.22	0.13	0.15
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	10	0.2	0.05	0.21
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	10	0.13	0.03	0.12
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	9	0.28	0.11	0.29
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	9	0.28	0.11	0.29
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	9	0.28	0.11	0.29
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	9	0.25	0.1	0.25
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	9	0.25	0.1	0.25
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	9	0.23	0.12	0.16
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	9	0.23	0.12	0.16
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	9	0.23	0.12	0.16
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	9	0.23	0.12	0.16
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	9	0.23	0.12	0.16
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	9	0.23	0.12	0.16
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	9	0.23	0.12	0.16
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	9	0.23	0.12	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	9	0.23	0.12	0.16
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	9	0.22	0.06	0.23
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	9	0.22	0.06	0.23
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	9	0.22	0.06	0.23
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	9	0.22	0.06	0.23
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	9	0.22	0.06	0.23
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	9	0.22	0.06	0.23
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	9	0.22	0.07	0.2
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	9	0.22	0.07	0.2
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	9	0.22	0.07	0.2
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	9	0.22	0.07	0.2
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	9	0.22	0.07	0.2
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	9	0.22	0.07	0.2
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	9	0.19	0.07	0.18
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	9	0.17	0.05	0.16
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	9	0.17	0.05	0.16
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	9	0.17	0.05	0.16
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	9	0.17	0.05	0.16
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	9	0.17	0.05	0.16
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	9	0.17	0.05	0.16
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	9	0.13	0.02	0.13
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	8	0.45	0.32	0.36
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	8	0.45	0.32	0.36
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	8	0.45	0.32	0.36
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	8	0.3	0.1	0.3
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	8	0.29	0.18	0.18
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	8	0.29	0.18	0.18
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	8	0.27	0.15	0.2
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	8	0.27	0.15	0.2
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	8	0.25	0.12	0.24
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	8	0.25	0.12	0.24
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	8	0.25	0.17	0.18
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	8	0.23	0.13	0.18
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	8	0.23	0.13	0.18
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	8	0.23	0.13	0.18
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	8	0.23	0.13	0.18
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	8	0.23	0.13	0.18
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	8	0.23	0.13	0.18
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	8	0.23	0.1	0.22
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	8	0.23	0.1	0.22
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	8	0.23	0.1	0.22
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	8	0.23	0.1	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	8	0.23	0.1	0.22
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	8	0.23	0.1	0.22
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	8	0.2	0.04	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	8	0.19	0.06	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	8	0.19	0.06	0.19
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	7	0.29	0.14	0.32
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	7	0.29	0.09	0.3
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	7	0.28	0.12	0.28
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	7	0.28	0.12	0.28
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	7	0.22	0.08	0.21
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	7	0.22	0.08	0.21
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	7	0.19	0.06	0.18
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	7	0.19	0.06	0.18
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	7	0.19	0.06	0.18
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	7	0.19	0.08	0.18
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	7	0.18	0.06	0.14
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	7	0.18	0.06	0.14
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	7	0.18	0.06	0.14
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	7	0.18	0.06	0.14
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	7	0.18	0.06	0.14
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	7	0.18	0.06	0.14
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	7	0.17	0.05	0.16
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	7	0.16	0.03	0.16
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	7	0.16	0.04	0.13
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	7	0.15	0.03	0.15
(1,115)	1:57:A:PHE:H	1:56:A:PHE:HA	6	0.32	0.04	0.32
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD11	6	0.32	0.24	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD12	6	0.32	0.24	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD13	6	0.32	0.24	0.17
(1,119)	1:57:A:PHE:H	1:57:A:PHE:HB2	6	0.26	0.09	0.22
(1,309)	1:118:A:ALA:HB1	1:115:A:TRP:HA	6	0.21	0.07	0.18
(1,309)	1:118:A:ALA:HB2	1:115:A:TRP:HA	6	0.21	0.07	0.18
(1,309)	1:118:A:ALA:HB3	1:115:A:TRP:HA	6	0.21	0.07	0.18
(1,243)	1:91:A:MET:H	1:88:A:ALA:HA	6	0.18	0.05	0.16
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD1	6	0.18	0.08	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD2	6	0.18	0.08	0.16
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD1	6	0.18	0.08	0.16
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD2	6	0.18	0.08	0.16
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD1	6	0.18	0.08	0.16
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD2	6	0.18	0.08	0.16
(1,73)	1:39:A:VAL:H	1:36:A:PHE:HA	6	0.17	0.05	0.18
(1,476)	1:171:A:VAL:H	1:168:A:ILE:HA	6	0.15	0.03	0.16
(1,504)	1:178:A:LEU:HD11	1:175:A:ILE:HA	6	0.15	0.04	0.14
(1,504)	1:178:A:LEU:HD12	1:175:A:ILE:HA	6	0.15	0.04	0.14
(1,504)	1:178:A:LEU:HD13	1:175:A:ILE:HA	6	0.15	0.04	0.14
(1,517)	1:183:A:PHE:H	1:180:A:LEU:HA	6	0.12	0.01	0.12
(1,335)	1:127:A:ILE:H	1:126:A:ALA:HA	6	0.11	0.0	0.11
(1,281)	1:111:A:LEU:H	1:111:A:LEU:HB2	5	0.54	0.28	0.72
(1,7)	1:5:A:PHE:H	1:5:A:PHE:HB2	5	0.48	0.1	0.55
(1,299)	1:114:A:LEU:H	1:114:A:LEU:HB3	5	0.46	0.27	0.41
(1,260)	1:105:A:PHE:H	1:105:A:PHE:HB3	5	0.41	0.2	0.44
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD11	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD12	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD13	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD21	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD22	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD23	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD11	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD12	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD13	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD21	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD22	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD23	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD11	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD12	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD13	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD21	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD22	5	0.39	0.18	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD23	5	0.39	0.18	0.42
(1,495)	1:175:A:ILE:HG21	1:172:A:THR:HA	5	0.33	0.17	0.32
(1,495)	1:175:A:ILE:HG22	1:172:A:THR:HA	5	0.33	0.17	0.32
(1,495)	1:175:A:ILE:HG23	1:172:A:THR:HA	5	0.33	0.17	0.32
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB2	5	0.3	0.13	0.36
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB3	5	0.3	0.13	0.36
(1,101)	1:49:A:LEU:H	1:49:A:LEU:HB3	5	0.24	0.09	0.26
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE2	5	0.21	0.1	0.19
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE3	5	0.21	0.1	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE2	5	0.21	0.1	0.19
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE3	5	0.21	0.1	0.19
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE2	5	0.21	0.1	0.19
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE3	5	0.21	0.1	0.19
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD11	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD12	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD13	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD11	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD12	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD13	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD11	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD12	5	0.2	0.07	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD13	5	0.2	0.07	0.24
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB1	5	0.19	0.07	0.19
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB2	5	0.19	0.07	0.19
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB3	5	0.19	0.07	0.19
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA2	5	0.18	0.08	0.19
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA3	5	0.18	0.08	0.19
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD2	5	0.17	0.05	0.16
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD3	5	0.17	0.05	0.16
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD2	5	0.17	0.05	0.16
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD3	5	0.17	0.05	0.16
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD2	5	0.17	0.05	0.16
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD3	5	0.17	0.05	0.16
(1,573)	1:88:A:ALA:HB1	1:76:A:LEU:HG	5	0.17	0.05	0.17
(1,573)	1:88:A:ALA:HB2	1:76:A:LEU:HG	5	0.17	0.05	0.17
(1,573)	1:88:A:ALA:HB3	1:76:A:LEU:HG	5	0.17	0.05	0.17
(1,116)	1:57:A:PHE:H	1:56:A:PHE:H	5	0.16	0.04	0.15
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG21	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG22	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG23	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG21	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG22	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG23	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG21	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG22	5	0.15	0.03	0.15
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG23	5	0.15	0.03	0.15
(1,423)	1:153:A:VAL:H	1:150:A:ILE:HA	5	0.12	0.02	0.12
(1,339)	1:128:A:SER:H	1:125:A:ILE:HA	5	0.12	0.01	0.12
(1,86)	1:42:A:LEU:H	1:41:A:GLY:HA2	5	0.11	0.01	0.11
(1,261)	1:105:A:PHE:H	1:105:A:PHE:HB2	4	0.41	0.13	0.48
(1,453)	1:165:A:PHE:H	1:165:A:PHE:HB2	4	0.36	0.24	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,107)	1:50:A:GLY:H	1:51:A:TYR:H	4	0.34	0.15	0.36
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB2	4	0.28	0.1	0.3
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB3	4	0.28	0.1	0.3
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB2	4	0.28	0.1	0.3
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB3	4	0.28	0.1	0.3
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB2	4	0.28	0.1	0.3
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB3	4	0.28	0.1	0.3
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE21	4	0.26	0.11	0.22
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE22	4	0.26	0.11	0.22
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE21	4	0.26	0.11	0.22
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE22	4	0.26	0.11	0.22
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE21	4	0.26	0.11	0.22
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE22	4	0.26	0.11	0.22
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE1	4	0.24	0.04	0.24
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE2	4	0.24	0.04	0.24
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE1	4	0.24	0.04	0.24
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE2	4	0.24	0.04	0.24
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE1	4	0.24	0.04	0.24
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE2	4	0.24	0.04	0.24
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG21	4	0.24	0.06	0.24
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG22	4	0.24	0.06	0.24
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG23	4	0.24	0.06	0.24
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD11	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD12	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD13	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD11	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD12	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD13	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD11	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD12	4	0.24	0.09	0.2
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD13	4	0.24	0.09	0.2
(1,589)	1:118:A:ALA:HB1	1:175:A:ILE:HA	4	0.21	0.09	0.2
(1,589)	1:118:A:ALA:HB2	1:175:A:ILE:HA	4	0.21	0.09	0.2
(1,589)	1:118:A:ALA:HB3	1:175:A:ILE:HA	4	0.21	0.09	0.2
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB1	4	0.18	0.03	0.18
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB2	4	0.18	0.03	0.18
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB3	4	0.18	0.03	0.18
(1,85)	1:42:A:LEU:H	1:39:A:VAL:HA	4	0.16	0.08	0.12
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD21	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD22	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD21	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD22	4	0.16	0.07	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD21	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD22	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD21	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD22	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD21	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD22	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD21	4	0.16	0.07	0.14
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD22	4	0.16	0.07	0.14
(1,607)	1:161:A:VAL:HG11	1:152:A:ALA:HA	4	0.16	0.05	0.16
(1,607)	1:161:A:VAL:HG12	1:152:A:ALA:HA	4	0.16	0.05	0.16
(1,607)	1:161:A:VAL:HG13	1:152:A:ALA:HA	4	0.16	0.05	0.16
(1,371)	1:140:A:LEU:H	1:137:A:LEU:H	4	0.15	0.04	0.14
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD1	4	0.15	0.03	0.15
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD2	4	0.15	0.03	0.15
(1,446)	1:163:A:ALA:H	1:162:A:LYS:H	4	0.14	0.02	0.14
(1,300)	1:114:A:LEU:H	1:114:A:LEU:HB2	3	0.64	0.08	0.67
(1,280)	1:111:A:LEU:H	1:111:A:LEU:HB3	3	0.41	0.25	0.31
(1,296)	1:114:A:LEU:H	1:111:A:LEU:HA	3	0.26	0.1	0.22
(1,289)	1:112:A:ALA:H	1:114:A:LEU:H	3	0.22	0.1	0.19
(1,462)	1:168:A:ILE:H	1:165:A:PHE:HA	3	0.21	0.05	0.18
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD11	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD12	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD13	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD11	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD12	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD13	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD11	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD12	3	0.21	0.07	0.25
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD13	3	0.21	0.07	0.25
(1,32)	1:12:A:VAL:H	1:9:A:ILE:HA	3	0.17	0.04	0.18
(1,447)	1:163:A:ALA:H	1:164:A:ASN:H	3	0.16	0.07	0.12
(1,448)	1:164:A:ASN:H	1:163:A:ALA:H	3	0.16	0.07	0.12
(1,210)	1:84:A:VAL:HG21	1:80:A:LEU:HA	3	0.16	0.05	0.14
(1,210)	1:84:A:VAL:HG22	1:80:A:LEU:HA	3	0.16	0.05	0.14
(1,210)	1:84:A:VAL:HG23	1:80:A:LEU:HA	3	0.16	0.05	0.14
(1,490)	1:174:A:ALA:H	1:171:A:VAL:HA	3	0.15	0.05	0.12
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG21	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG22	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG23	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG21	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG22	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG23	3	0.14	0.0	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG21	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG22	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG23	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG21	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG22	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG23	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG21	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG22	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG23	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG21	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG22	3	0.14	0.0	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG23	3	0.14	0.0	0.14
(1,393)	1:145:A:GLY:H	1:144:A:LEU:HA	3	0.12	0.0	0.12
(1,531)	1:16:A:ALA:HB1	1:27:A:GLY:H	3	0.11	0.01	0.11
(1,531)	1:16:A:ALA:HB2	1:27:A:GLY:H	3	0.11	0.01	0.11
(1,531)	1:16:A:ALA:HB3	1:27:A:GLY:H	3	0.11	0.01	0.11
(1,402)	1:148:A:VAL:H	1:147:A:ALA:HA	3	0.11	0.01	0.1
(1,563)	1:66:A:LEU:HD11	1:113:A:PHE:HD1	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD11	1:113:A:PHE:HD2	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD12	1:113:A:PHE:HD1	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD12	1:113:A:PHE:HD2	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD13	1:113:A:PHE:HD1	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD13	1:113:A:PHE:HD2	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD21	1:113:A:PHE:HD1	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD21	1:113:A:PHE:HD2	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD22	1:113:A:PHE:HD1	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD22	1:113:A:PHE:HD2	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD23	1:113:A:PHE:HD1	2	0.52	0.25	0.52
(1,563)	1:66:A:LEU:HD23	1:113:A:PHE:HD2	2	0.52	0.25	0.52
(1,6)	1:5:A:PHE:H	1:5:A:PHE:HB3	2	0.48	0.12	0.48
(1,591)	1:119:A:ILE:HD11	1:25:A:PHE:HE1	2	0.38	0.01	0.38
(1,591)	1:119:A:ILE:HD11	1:25:A:PHE:HE2	2	0.38	0.01	0.38
(1,591)	1:119:A:ILE:HD12	1:25:A:PHE:HE1	2	0.38	0.01	0.38
(1,591)	1:119:A:ILE:HD12	1:25:A:PHE:HE2	2	0.38	0.01	0.38
(1,591)	1:119:A:ILE:HD13	1:25:A:PHE:HE1	2	0.38	0.01	0.38
(1,591)	1:119:A:ILE:HD13	1:25:A:PHE:HE2	2	0.38	0.01	0.38
(1,541)	1:38:A:ILE:HD11	1:67:A:PHE:HE1	2	0.36	0.08	0.36
(1,541)	1:38:A:ILE:HD11	1:67:A:PHE:HE2	2	0.36	0.08	0.36
(1,541)	1:38:A:ILE:HD12	1:67:A:PHE:HE1	2	0.36	0.08	0.36
(1,541)	1:38:A:ILE:HD12	1:67:A:PHE:HE2	2	0.36	0.08	0.36
(1,541)	1:38:A:ILE:HD13	1:67:A:PHE:HE1	2	0.36	0.08	0.36
(1,541)	1:38:A:ILE:HD13	1:67:A:PHE:HE2	2	0.36	0.08	0.36

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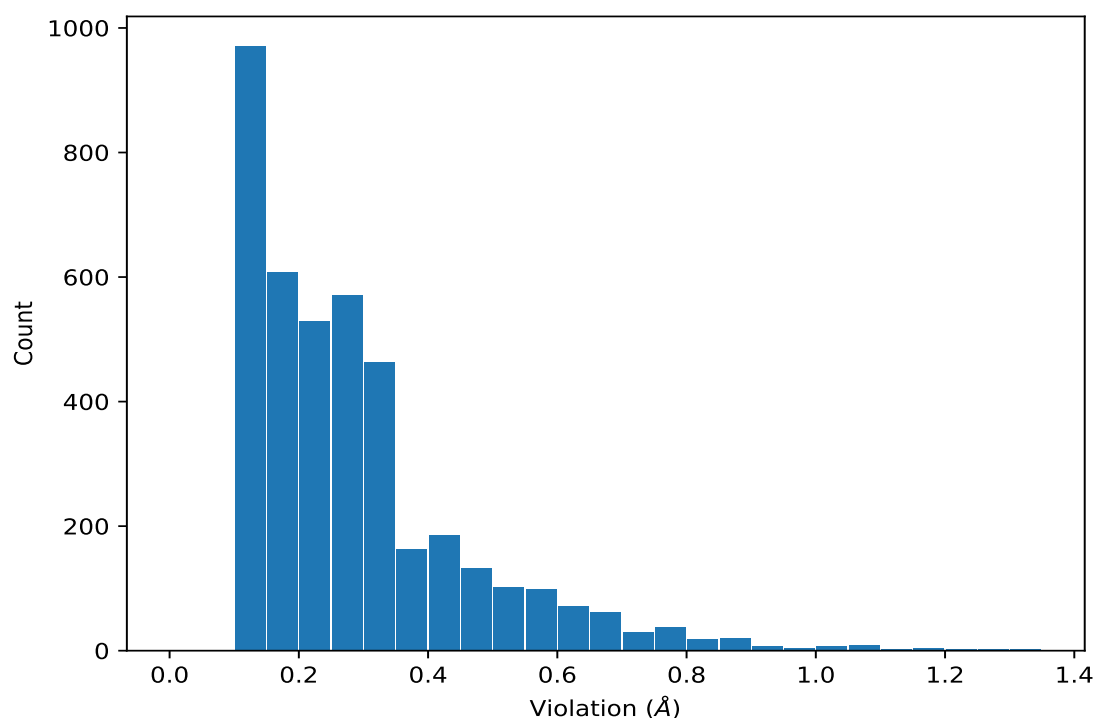
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,113)	1:56:A:PHE:H	1:56:A:PHE:HB2	2	0.3	0.16	0.3
(1,194)	1:79:A:GLU:H	1:78:A:ASP:HA	2	0.26	0.0	0.26
(1,559)	1:50:A:GLY:H	1:182:A:TYR:HE1	2	0.24	0.12	0.24
(1,559)	1:50:A:GLY:H	1:182:A:TYR:HE2	2	0.24	0.12	0.24
(1,262)	1:106:A:PHE:H	1:105:A:PHE:H	2	0.24	0.1	0.24
(1,209)	1:84:A:VAL:HG11	1:82:A:GLU:H	2	0.21	0.05	0.21
(1,209)	1:84:A:VAL:HG12	1:82:A:GLU:H	2	0.21	0.05	0.21
(1,209)	1:84:A:VAL:HG13	1:82:A:GLU:H	2	0.21	0.05	0.21
(1,576)	1:110:A:LEU:HD21	1:105:A:PHE:HD1	2	0.21	0.05	0.21
(1,576)	1:110:A:LEU:HD21	1:105:A:PHE:HD2	2	0.21	0.05	0.21
(1,576)	1:110:A:LEU:HD22	1:105:A:PHE:HD1	2	0.21	0.05	0.21
(1,576)	1:110:A:LEU:HD22	1:105:A:PHE:HD2	2	0.21	0.05	0.21
(1,576)	1:110:A:LEU:HD23	1:105:A:PHE:HD1	2	0.21	0.05	0.21
(1,576)	1:110:A:LEU:HD23	1:105:A:PHE:HD2	2	0.21	0.05	0.21
(1,327)	1:125:A:ILE:HD11	1:122:A:PHE:HD1	2	0.2	0.01	0.2
(1,327)	1:125:A:ILE:HD11	1:122:A:PHE:HD2	2	0.2	0.01	0.2
(1,327)	1:125:A:ILE:HD12	1:122:A:PHE:HD1	2	0.2	0.01	0.2
(1,327)	1:125:A:ILE:HD12	1:122:A:PHE:HD2	2	0.2	0.01	0.2
(1,327)	1:125:A:ILE:HD13	1:122:A:PHE:HD1	2	0.2	0.01	0.2
(1,327)	1:125:A:ILE:HD13	1:122:A:PHE:HD2	2	0.2	0.01	0.2
(1,485)	1:172:A:THR:H	1:174:A:ALA:H	2	0.19	0.03	0.19
(1,225)	1:87:A:PHE:H	1:87:A:PHE:HB2	2	0.15	0.05	0.15
(1,534)	1:24:A:ILE:HD11	1:17:A:VAL:HB	2	0.15	0.0	0.15
(1,534)	1:24:A:ILE:HD12	1:17:A:VAL:HB	2	0.15	0.0	0.15
(1,534)	1:24:A:ILE:HD13	1:17:A:VAL:HB	2	0.15	0.0	0.15
(1,166)	1:72:A:ALA:H	1:74:A:ILE:H	2	0.14	0.02	0.14
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB1	2	0.12	0.01	0.12
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB2	2	0.12	0.01	0.12
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB3	2	0.12	0.01	0.12
(1,305)	1:115:A:TRP:H	1:116:A:LEU:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	10	1.31
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	9	1.3
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	15	1.29
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	2	1.28
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	12	1.22
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	14	1.21
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	4	1.2
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	11	1.19
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	2	1.17
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	1	1.16
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	9	1.12
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	13	1.11
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	7	1.09
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	7	1.09
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	13	1.09
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	13	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	8	1.07
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	14	1.07
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	5	1.07
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	6	1.07
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	8	1.05
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	7	1.04
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	11	1.04
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	4	1.02
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	1	1.01
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	5	1.0
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	5	1.0
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	5	1.0
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	1	0.99
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	1	0.99
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	12	0.96
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	12	0.96
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	6	0.95
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	6	0.95
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	15	0.95
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	15	0.95
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	13	0.94
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	3	0.93
(1,308)	1:118:A:ALA:H	1:119:A:ILE:H	10	0.93
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	15	0.88
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	15	0.88
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	15	0.88
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	8	0.87
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	8	0.87
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	11	0.87
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	11	0.87
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	11	0.87
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	11	0.87
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	11	0.87
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	11	0.87
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	11	0.87
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	11	0.87
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	11	0.87
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	5	0.87
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	5	0.87
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	15	0.87
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	15	0.87
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	3	0.87
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	4	0.85
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	4	0.85
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	5	0.84
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	5	0.84
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	8	0.84
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	8	0.84
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	14	0.84
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	14	0.84
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	3	0.83
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	3	0.83
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	15	0.83
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	15	0.83
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	7	0.82
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	7	0.82
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	10	0.81
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	10	0.81
(1,281)	1:111:A:LEU:H	1:111:A:LEU:HB2	11	0.81
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	9	0.8
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	9	0.8
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	14	0.79
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	14	0.79
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	2	0.79
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	2	0.79
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	11	0.79
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	11	0.79
(1,299)	1:114:A:LEU:H	1:114:A:LEU:HB3	9	0.79
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	6	0.78
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	6	0.78
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	6	0.78
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	6	0.78
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	7	0.78
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	7	0.78
(1,281)	1:111:A:LEU:H	1:111:A:LEU:HB2	6	0.78
(1,563)	1:66:A:LEU:HD11	1:113:A:PHE:HD1	11	0.77
(1,563)	1:66:A:LEU:HD11	1:113:A:PHE:HD2	11	0.77
(1,563)	1:66:A:LEU:HD12	1:113:A:PHE:HD1	11	0.77
(1,563)	1:66:A:LEU:HD12	1:113:A:PHE:HD2	11	0.77
(1,563)	1:66:A:LEU:HD13	1:113:A:PHE:HD1	11	0.77
(1,563)	1:66:A:LEU:HD13	1:113:A:PHE:HD2	11	0.77
(1,563)	1:66:A:LEU:HD21	1:113:A:PHE:HD1	11	0.77
(1,563)	1:66:A:LEU:HD21	1:113:A:PHE:HD2	11	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:66:A:LEU:HD22	1:113:A:PHE:HD1	11	0.77
(1,563)	1:66:A:LEU:HD22	1:113:A:PHE:HD2	11	0.77
(1,563)	1:66:A:LEU:HD23	1:113:A:PHE:HD1	11	0.77
(1,563)	1:66:A:LEU:HD23	1:113:A:PHE:HD2	11	0.77
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	3	0.77
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	14	0.77
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	3	0.76
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	3	0.76
(1,280)	1:111:A:LEU:H	1:111:A:LEU:HB3	12	0.76
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	10	0.75
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	10	0.75
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	13	0.75
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	13	0.75
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	8	0.75
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	12	0.75
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	2	0.74
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	2	0.74
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	2	0.74
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	4	0.74
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	4	0.74
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	2	0.74
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG2	9	0.74
(1,322)	1:124:A:GLY:H	1:121:A:PRO:HG3	9	0.74
(1,299)	1:114:A:LEU:H	1:114:A:LEU:HB3	6	0.74
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	1	0.73
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	1	0.73
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	13	0.73
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	12	0.72
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	12	0.72
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	12	0.72
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	12	0.72
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	12	0.72
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	12	0.72
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	8	0.72
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	8	0.72
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	1	0.72
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	1	0.72
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	8	0.72
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	8	0.72
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	5	0.72
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	7	0.72
(1,300)	1:114:A:LEU:H	1:114:A:LEU:HB2	10	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:111:A:LEU:H	1:111:A:LEU:HB2	13	0.72
(1,260)	1:105:A:PHE:H	1:105:A:PHE:HB3	5	0.72
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	15	0.71
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	12	0.7
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	12	0.7
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD11	13	0.7
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD12	13	0.7
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD13	13	0.7
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	3	0.7
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	3	0.7
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	3	0.7
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	3	0.7
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	3	0.7
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	3	0.7
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	10	0.7
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	10	0.7
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	10	0.7
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	10	0.7
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	10	0.7
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	10	0.7
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	15	0.7
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	11	0.69
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	11	0.69
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	11	0.69
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	11	0.69
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	11	0.69
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	11	0.69
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	3	0.69
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	3	0.69
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	3	0.69
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	4	0.69
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	15	0.68
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	12	0.68
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	14	0.67
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	14	0.67
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	12	0.67
(1,300)	1:114:A:LEU:H	1:114:A:LEU:HB2	3	0.67
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	15	0.66
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	15	0.66
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	12	0.66
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	12	0.66
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	6	0.66
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	6	0.66
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	10	0.66
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	7	0.66
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	7	0.65
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	7	0.65
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	7	0.65
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	7	0.65
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	7	0.65
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	7	0.65
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	1	0.65
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	1	0.65
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	1	0.65
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	8	0.65
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	8	0.65
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	8	0.65
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	2	0.65
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	2	0.65
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	1	0.65
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	1	0.65
(1,495)	1:175:A:ILE:HG21	1:172:A:THR:HA	4	0.65
(1,495)	1:175:A:ILE:HG22	1:172:A:THR:HA	4	0.65
(1,495)	1:175:A:ILE:HG23	1:172:A:THR:HA	4	0.65
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	1	0.64
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	1	0.64
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	1	0.64
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	1	0.64
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	1	0.64
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	1	0.64
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	3	0.63
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	3	0.63
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	9	0.63
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	9	0.63
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	9	0.63
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	9	0.63
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	9	0.63
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	9	0.63
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	8	0.63
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	8	0.63
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	8	0.63
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	8	0.63
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	8	0.63
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	8	0.63
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	8	0.63
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	8	0.63
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	15	0.63
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	15	0.63
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	4	0.63
(1,383)	1:142:A:TYR:H	1:142:A:TYR:HB3	10	0.63
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	4	0.62
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	4	0.62
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD11	12	0.62
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD12	12	0.62
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD13	12	0.62
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	12	0.62
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	12	0.62
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	13	0.62
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	13	0.62
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	10	0.61
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	10	0.61
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	5	0.61
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	5	0.61
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	5	0.61
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	5	0.61
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	5	0.61
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	5	0.61
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	12	0.61
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	12	0.61
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	15	0.61
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	15	0.61
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	15	0.61
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	15	0.61
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	15	0.61
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	15	0.61
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	9	0.61
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	6	0.61
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	6	0.61
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	6	0.61
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	6	0.61
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	6	0.61
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	6	0.61
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	6	0.61
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	6	0.61
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD1	11	0.61
(1,553)	1:46:A:MET:H	1:60:A:PHE:HD2	11	0.61
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	10	0.61
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	10	0.61
(1,453)	1:165:A:PHE:H	1:165:A:PHE:HB2	8	0.61
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	2	0.61
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	9	0.61
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	10	0.61
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	12	0.61
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	5	0.6
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	5	0.6
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	5	0.6
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	6	0.6
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	13	0.6
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	3	0.6
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	4	0.6
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	5	0.6
(1,6)	1:5:A:PHE:H	1:5:A:PHE:HB3	8	0.6
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD11	11	0.59
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD12	11	0.59
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD13	11	0.59
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD21	11	0.59
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD22	11	0.59
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD23	11	0.59
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD11	11	0.59
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD12	11	0.59
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD13	11	0.59
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD21	11	0.59
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD22	11	0.59
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD23	11	0.59
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD11	11	0.59
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD12	11	0.59
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD13	11	0.59
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD21	11	0.59
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD22	11	0.59
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD23	11	0.59
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	5	0.59
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	8	0.59
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	15	0.59
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	9	0.59
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	5	0.58
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	7	0.58
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	7	0.58
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	12	0.58
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	12	0.58
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	12	0.58
(1,453)	1:165:A:PHE:H	1:165:A:PHE:HB2	9	0.58
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	3	0.58
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	10	0.58
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	8	0.58
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	1	0.58
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	14	0.58
(1,7)	1:5:A:PHE:H	1:5:A:PHE:HB2	11	0.58
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	3	0.57
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	3	0.57
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	1	0.57
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	1	0.57
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	14	0.57
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	14	0.57
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	14	0.57
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	3	0.57
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	3	0.57
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	1	0.57
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	15	0.57
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	4	0.57
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	4	0.57
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	4	0.57
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	10	0.57
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	7	0.56
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	11	0.56
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	15	0.56
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	15	0.56
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	9	0.56
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	9	0.56
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	9	0.56
(1,7)	1:5:A:PHE:H	1:5:A:PHE:HB2	12	0.56
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	11	0.55
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	11	0.55
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	13	0.55
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	13	0.55
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	11	0.55
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	11	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	1	0.55
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD11	15	0.55
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD12	15	0.55
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD13	15	0.55
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD21	15	0.55
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD22	15	0.55
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD23	15	0.55
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD11	15	0.55
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD12	15	0.55
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD13	15	0.55
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD21	15	0.55
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD22	15	0.55
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD23	15	0.55
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD11	15	0.55
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD12	15	0.55
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD13	15	0.55
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD21	15	0.55
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD22	15	0.55
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD23	15	0.55
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	5	0.55
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	6	0.55
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	6	0.55
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	6	0.55
(1,7)	1:5:A:PHE:H	1:5:A:PHE:HB2	5	0.55
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	4	0.54
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	4	0.54
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	4	0.54
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	4	0.54
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	4	0.54
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	4	0.54
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	13	0.54
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	13	0.54
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	13	0.54
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	13	0.54
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	13	0.54
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	13	0.54
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	9	0.54
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	9	0.54
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	9	0.54
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	9	0.54
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	9	0.54
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	9	0.54
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	9	0.54
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	9	0.54
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	14	0.54
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	14	0.54
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	14	0.54
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	14	0.54
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	14	0.54
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	14	0.54
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	5	0.54
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	5	0.54
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	6	0.54
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	6	0.54
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	14	0.54
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	7	0.54
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	4	0.54
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	11	0.53
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	11	0.53
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	10	0.53
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	10	0.53
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	10	0.53
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	9	0.53
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	12	0.53
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	15	0.53
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	7	0.53
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	7	0.53
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	7	0.53
(1,224)	1:87:A:PHE:H	1:87:A:PHE:HB3	15	0.53
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	14	0.53
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	11	0.52
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	11	0.52
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	11	0.52
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	2	0.52
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	2	0.52
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	2	0.52
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	2	0.52
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	2	0.52
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	2	0.52
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	2	0.52
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	2	0.52
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	2	0.52
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	5	0.52
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	5	0.52
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	5	0.52
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	5	0.52
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	5	0.52
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	11	0.52
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	11	0.52
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	11	0.52
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	11	0.52
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	11	0.52
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	11	0.52
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	13	0.52
(1,300)	1:114:A:LEU:H	1:114:A:LEU:HB2	14	0.52
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	12	0.52
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	6	0.52
(1,107)	1:50:A:GLY:H	1:51:A:TYR:H	15	0.52
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	13	0.52
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	13	0.52
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	13	0.52
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	9	0.52
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	2	0.51
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	14	0.51
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	12	0.51
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	12	0.51
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	2	0.51
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	2	0.51
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	2	0.51
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	8	0.51
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	11	0.51
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	13	0.51
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	2	0.5
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	2	0.5
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	2	0.5
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	2	0.5
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	2	0.5
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	2	0.5
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	15	0.5
(1,261)	1:105:A:PHE:H	1:105:A:PHE:HB2	11	0.5
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	2	0.5
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	2	0.5
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	2	0.5
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	5	0.49
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	5	0.49
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	2	0.49
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	2	0.49
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	2	0.49
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	2	0.49
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	2	0.49
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	2	0.49
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	4	0.49
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	4	0.49
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	4	0.49
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	10	0.49
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	10	0.49
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	8	0.49
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	8	0.49
(1,196)	1:80:A:LEU:H	1:79:A:GLU:HA	5	0.49
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	15	0.49
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	3	0.49
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	13	0.49
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	13	0.49
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	13	0.49
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	14	0.48
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	14	0.48
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	14	0.48
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	14	0.48
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	14	0.48
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	14	0.48
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	9	0.48
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	9	0.48
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	1	0.48
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	1	0.48
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	15	0.48
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	15	0.48
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	15	0.48
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	15	0.48
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	15	0.48
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	15	0.48
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	5	0.48
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	11	0.48
(1,261)	1:105:A:PHE:H	1:105:A:PHE:HB2	3	0.48
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	10	0.48
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	12	0.48
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	10	0.48
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	10	0.48
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	10	0.48
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	4	0.48
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	12	0.47
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	12	0.47
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	12	0.47
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB2	4	0.47
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB3	4	0.47
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	13	0.47
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	13	0.47
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	13	0.47
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	13	0.47
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	13	0.47
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	13	0.47
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	13	0.47
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	13	0.47
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	13	0.47
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	11	0.47
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	11	0.47
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	7	0.47
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	12	0.47
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	9	0.47
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	9	0.47
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	9	0.47
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	1	0.47
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	7	0.47
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	13	0.47
(1,261)	1:105:A:PHE:H	1:105:A:PHE:HB2	9	0.47
(1,260)	1:105:A:PHE:H	1:105:A:PHE:HB3	2	0.47
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	6	0.47
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	2	0.46
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	2	0.46
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	11	0.46
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	11	0.46
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	10	0.46
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	12	0.46
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	12	0.46
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	12	0.46
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	12	0.46
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	12	0.46
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	12	0.46
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	12	0.46
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	12	0.46
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	2	0.46
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	2	0.46
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	6	0.46
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	4	0.46
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	6	0.46
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	8	0.46
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	10	0.46
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	13	0.46
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	7	0.46
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	7	0.46
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	7	0.46
(1,113)	1:56:A:PHE:H	1:56:A:PHE:HB2	15	0.46
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	8	0.46
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	12	0.46
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	7	0.45
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	7	0.45
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	10	0.45
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	10	0.45
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	4	0.45
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	4	0.45
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	14	0.45
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	14	0.45
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	3	0.45
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	14	0.45
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	14	0.45
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	14	0.45
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	14	0.45
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	14	0.45
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	14	0.45
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	15	0.45
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	15	0.45
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	7	0.45
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	7	0.45
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	2	0.45
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	14	0.45
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	2	0.45
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	12	0.45
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	12	0.45
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	12	0.45
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	12	0.45
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	12	0.45
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	12	0.45
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	12	0.45
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	12	0.45
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	5	0.44
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	5	0.44
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	7	0.44
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	7	0.44
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	9	0.44
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	9	0.44
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	15	0.44
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	15	0.44
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	14	0.44
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	14	0.44
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	5	0.44
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	5	0.44
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	4	0.44
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	4	0.44
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	4	0.44
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	4	0.44
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	4	0.44
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	4	0.44
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	4	0.44
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	4	0.44
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	4	0.44
(1,541)	1:38:A:ILE:HD11	1:67:A:PHE:HE1	13	0.44
(1,541)	1:38:A:ILE:HD11	1:67:A:PHE:HE2	13	0.44
(1,541)	1:38:A:ILE:HD12	1:67:A:PHE:HE1	13	0.44
(1,541)	1:38:A:ILE:HD12	1:67:A:PHE:HE2	13	0.44
(1,541)	1:38:A:ILE:HD13	1:67:A:PHE:HE1	13	0.44
(1,541)	1:38:A:ILE:HD13	1:67:A:PHE:HE2	13	0.44
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	3	0.44
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	1	0.44
(1,452)	1:165:A:PHE:H	1:165:A:PHE:HB3	2	0.44
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	5	0.44
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	7	0.44
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE21	3	0.44
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE22	3	0.44
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE21	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE22	3	0.44
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE21	3	0.44
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE22	3	0.44
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	2	0.44
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	3	0.44
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	9	0.44
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	14	0.44
(1,260)	1:105:A:PHE:H	1:105:A:PHE:HB3	10	0.44
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	1	0.44
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	2	0.44
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	13	0.44
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	4	0.43
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	4	0.43
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	4	0.43
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	4	0.43
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	4	0.43
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	4	0.43
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	6	0.43
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	6	0.43
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	11	0.43
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	11	0.43
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	11	0.43
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	11	0.43
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	11	0.43
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	11	0.43
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	11	0.43
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	11	0.43
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	11	0.43
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	13	0.43
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	13	0.43
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	5	0.43
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	11	0.43
(1,312)	1:123:A:ALA:H	1:122:A:PHE:HA	12	0.43
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	15	0.43
(1,294)	1:113:A:PHE:H	1:113:A:PHE:HB2	2	0.43
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	3	0.43
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	9	0.43
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	6	0.43
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	5	0.43
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	5	0.43
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	8	0.43
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	15	0.43
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	14	0.42
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	14	0.42
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	7	0.42
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	7	0.42
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	7	0.42
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	11	0.42
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	8	0.42
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	8	0.42
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	14	0.42
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	14	0.42
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	14	0.42
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	14	0.42
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	14	0.42
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	14	0.42
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	14	0.42
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	14	0.42
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	14	0.42
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	4	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD11	12	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD12	12	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD13	12	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD21	12	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD22	12	0.42
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD23	12	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD11	12	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD12	12	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD13	12	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD21	12	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD22	12	0.42
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD23	12	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD11	12	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD12	12	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD13	12	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD21	12	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD22	12	0.42
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD23	12	0.42
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	1	0.42
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	14	0.42
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	13	0.42
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	13	0.42
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	11	0.42
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	11	0.42
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	11	0.42
(1,107)	1:50:A:GLY:H	1:51:A:TYR:H	3	0.42
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	15	0.41
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	15	0.41
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	13	0.41
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	13	0.41
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	13	0.41
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	13	0.41
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	13	0.41
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	13	0.41
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	10	0.41
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	10	0.41
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	14	0.41
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	14	0.41
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	14	0.41
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	14	0.41
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	14	0.41
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	14	0.41
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	4	0.41
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	4	0.41
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	4	0.41
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	4	0.41
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	4	0.41
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	4	0.41
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	15	0.41
(1,299)	1:114:A:LEU:H	1:114:A:LEU:HB3	10	0.41
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	13	0.41
(1,115)	1:57:A:PHE:H	1:56:A:PHE:HA	15	0.41
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	9	0.41
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	9	0.41
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	9	0.41
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	9	0.41
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	9	0.41
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	9	0.41
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	9	0.41
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	9	0.41
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	9	0.41
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	1	0.4
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	1	0.4
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	12	0.4
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	12	0.4
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	12	0.4
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	12	0.4
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	12	0.4
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	12	0.4
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	12	0.4
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	12	0.4
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	3	0.4
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	10	0.4
(1,449)	1:164:A:ASN:H	1:165:A:PHE:H	6	0.4
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	7	0.4
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	1	0.4
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	1	0.4
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	1	0.4
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	2	0.4
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	2	0.4
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	2	0.4
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	10	0.4
(1,119)	1:57:A:PHE:H	1:57:A:PHE:HB2	5	0.4
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	9	0.4
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	14	0.4
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	1	0.4
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	1	0.4
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	3	0.4
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	2	0.39
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	2	0.39
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	13	0.39
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	13	0.39
(1,591)	1:119:A:ILE:HD11	1:25:A:PHE:HE1	7	0.39
(1,591)	1:119:A:ILE:HD11	1:25:A:PHE:HE2	7	0.39
(1,591)	1:119:A:ILE:HD12	1:25:A:PHE:HE1	7	0.39
(1,591)	1:119:A:ILE:HD12	1:25:A:PHE:HE2	7	0.39
(1,591)	1:119:A:ILE:HD13	1:25:A:PHE:HE1	7	0.39
(1,591)	1:119:A:ILE:HD13	1:25:A:PHE:HE2	7	0.39
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	8	0.39
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	13	0.39
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	13	0.39
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	13	0.39
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE2	14	0.39
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE3	14	0.39
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE2	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE3	14	0.39
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE2	14	0.39
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE3	14	0.39
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	9	0.39
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	9	0.39
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	10	0.39
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	3	0.39
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	10	0.39
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	12	0.39
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	4	0.39
(1,296)	1:114:A:LEU:H	1:111:A:LEU:HA	10	0.39
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	2	0.39
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	13	0.39
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	13	0.39
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	13	0.39
(1,31)	1:11:A:SER:H	1:13:A:PHE:H	7	0.39
(1,7)	1:5:A:PHE:H	1:5:A:PHE:HB2	4	0.39
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	11	0.38
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	11	0.38
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB2	13	0.38
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB3	13	0.38
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	15	0.38
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	15	0.38
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	15	0.38
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	15	0.38
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	15	0.38
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	15	0.38
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	15	0.38
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	15	0.38
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	15	0.38
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	2	0.38
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	2	0.38
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD11	11	0.38
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD12	11	0.38
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD13	11	0.38
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD11	11	0.38
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD12	11	0.38
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD13	11	0.38
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD11	11	0.38
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD12	11	0.38
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD13	11	0.38
(1,498)	1:176:A:VAL:H	1:173:A:GLY:HA2	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	15	0.38
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	8	0.38
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	8	0.38
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB2	15	0.38
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB3	15	0.38
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB2	15	0.38
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB3	15	0.38
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB2	15	0.38
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB3	15	0.38
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	10	0.38
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	6	0.38
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	5	0.37
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	5	0.37
(1,591)	1:119:A:ILE:HD11	1:25:A:PHE:HE1	15	0.37
(1,591)	1:119:A:ILE:HD11	1:25:A:PHE:HE2	15	0.37
(1,591)	1:119:A:ILE:HD12	1:25:A:PHE:HE1	15	0.37
(1,591)	1:119:A:ILE:HD12	1:25:A:PHE:HE2	15	0.37
(1,591)	1:119:A:ILE:HD13	1:25:A:PHE:HE1	15	0.37
(1,591)	1:119:A:ILE:HD13	1:25:A:PHE:HE2	15	0.37
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	14	0.37
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	14	0.37
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	14	0.37
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	5	0.37
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	5	0.37
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	8	0.37
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	8	0.37
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	8	0.37
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	8	0.37
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	8	0.37
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	8	0.37
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	8	0.37
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	8	0.37
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	8	0.37
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	12	0.37
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	5	0.37
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	8	0.37
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	9	0.36
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	9	0.36
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	2	0.36
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	2	0.36
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	2	0.36
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	5	0.36
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	5	0.36
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	15	0.36
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	15	0.36
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	3	0.36
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	3	0.36
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	3	0.36
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	3	0.36
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	3	0.36
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	3	0.36
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	10	0.36
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	10	0.36
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	6	0.36
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	6	0.36
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	14	0.36
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	14	0.36
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	15	0.36
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	15	0.36
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	15	0.36
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	15	0.36
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	15	0.36
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	15	0.36
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB2	3	0.36
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB3	3	0.36
(1,559)	1:50:A:GLY:H	1:182:A:TYR:HE1	6	0.36
(1,559)	1:50:A:GLY:H	1:182:A:TYR:HE2	6	0.36
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	10	0.36
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	10	0.36
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	10	0.36
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	10	0.36
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	10	0.36
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	10	0.36
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	13	0.36
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	13	0.36
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	13	0.36
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	13	0.36
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	13	0.36
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	13	0.36
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	11	0.36
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	11	0.36
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	11	0.36
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	11	0.36
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	11	0.36
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	11	0.36
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	11	0.36
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	11	0.36
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	15	0.36
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	6	0.36
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	12	0.36
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	14	0.36
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	14	0.36
(1,119)	1:57:A:PHE:H	1:57:A:PHE:HB2	4	0.36
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	13	0.36
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	11	0.36
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	11	0.36
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	11	0.36
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	4	0.36
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	4	0.36
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	4	0.36
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	9	0.36
(1,6)	1:5:A:PHE:H	1:5:A:PHE:HB3	13	0.36
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	4	0.35
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	4	0.35
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	14	0.35
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	14	0.35
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	14	0.35
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	14	0.35
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	14	0.35
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	14	0.35
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	3	0.35
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	3	0.35
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	3	0.35
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	3	0.35
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	10	0.35
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	10	0.35
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	15	0.35
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	7	0.35
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	7	0.35
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	7	0.35
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	7	0.35
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	7	0.35
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	7	0.35
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	2	0.35
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB2	8	0.35
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB3	8	0.35
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB2	8	0.35
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB3	8	0.35
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB2	8	0.35
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB3	8	0.35
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	6	0.35
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	14	0.35
(1,309)	1:118:A:ALA:HB1	1:115:A:TRP:HA	15	0.35
(1,309)	1:118:A:ALA:HB2	1:115:A:TRP:HA	15	0.35
(1,309)	1:118:A:ALA:HB3	1:115:A:TRP:HA	15	0.35
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	10	0.35
(1,289)	1:112:A:ALA:H	1:114:A:LEU:H	10	0.35
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	7	0.35
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	5	0.35
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	6	0.35
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	6	0.35
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	9	0.35
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	6	0.34
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	6	0.34
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	5	0.34
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	5	0.34
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	5	0.34
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	15	0.34
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	15	0.34
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	15	0.34
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	10	0.34
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	10	0.34
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	10	0.34
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	10	0.34
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	10	0.34
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	10	0.34
(1,589)	1:118:A:ALA:HB1	1:175:A:ILE:HA	15	0.34
(1,589)	1:118:A:ALA:HB2	1:175:A:ILE:HA	15	0.34
(1,589)	1:118:A:ALA:HB3	1:175:A:ILE:HA	15	0.34
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	2	0.34
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	2	0.34
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	2	0.34
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	2	0.34
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	2	0.34
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	2	0.34
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	2	0.34
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	2	0.34
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	7	0.34
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	7	0.34
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	7	0.34
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	7	0.34
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	7	0.34
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	7	0.34
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	7	0.34
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	7	0.34
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	7	0.34
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	9	0.34
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	9	0.34
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	9	0.34
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	1	0.34
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	1	0.34
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	1	0.34
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	1	0.34
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	1	0.34
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	1	0.34
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	11	0.34
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	11	0.34
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	11	0.34
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	11	0.34
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	11	0.34
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	11	0.34
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	1	0.34
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	1	0.34
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	1	0.34
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	6	0.34
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	13	0.34
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	13	0.34
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	13	0.34
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	13	0.34
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	13	0.34
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	13	0.34
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	9	0.34
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	9	0.34
(1,549)	1:42:A:LEU:HD11	1:182:A:TYR:HE1	6	0.34
(1,549)	1:42:A:LEU:HD11	1:182:A:TYR:HE2	6	0.34
(1,549)	1:42:A:LEU:HD12	1:182:A:TYR:HE1	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,549)	1:42:A:LEU:HD12	1:182:A:TYR:HE2	6	0.34
(1,549)	1:42:A:LEU:HD13	1:182:A:TYR:HE1	6	0.34
(1,549)	1:42:A:LEU:HD13	1:182:A:TYR:HE2	6	0.34
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	4	0.34
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	4	0.34
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	2	0.34
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	2	0.34
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	2	0.34
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	2	0.34
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	2	0.34
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	2	0.34
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	2	0.34
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	2	0.34
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	2	0.34
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	7	0.34
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	7	0.34
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	7	0.34
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	7	0.34
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	7	0.34
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	7	0.34
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	7	0.34
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	7	0.34
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	7	0.34
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	8	0.34
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	8	0.34
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	6	0.34
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD1	1	0.34
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD2	1	0.34
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD1	1	0.34
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD2	1	0.34
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD1	1	0.34
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD2	1	0.34
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	6	0.34
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	6	0.34
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	6	0.34
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	12	0.34
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	12	0.34
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	12	0.34
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	8	0.34
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	3	0.34
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	3	0.34
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	2	0.34
(1,101)	1:49:A:LEU:H	1:49:A:LEU:HB3	1	0.34
(1,101)	1:49:A:LEU:H	1:49:A:LEU:HB3	11	0.34
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	7	0.34
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	7	0.34
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	7	0.34
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	7	0.34
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	7	0.34
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	7	0.34
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	11	0.34
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	11	0.34
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	11	0.34
(1,7)	1:5:A:PHE:H	1:5:A:PHE:HB2	13	0.34
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	2	0.33
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	2	0.33
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	2	0.33
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	6	0.33
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	6	0.33
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	15	0.33
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	15	0.33
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	15	0.33
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	15	0.33
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	15	0.33
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	15	0.33
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	1	0.33
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	1	0.33
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	1	0.33
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	1	0.33
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	1	0.33
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	1	0.33
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	1	0.33
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	1	0.33
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	1	0.33
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	8	0.33
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	8	0.33
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	8	0.33
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	8	0.33
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	8	0.33
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	8	0.33
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	8	0.33
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	8	0.33
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	4	0.33
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	4	0.33
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	4	0.33
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	4	0.33
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	4	0.33
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	5	0.33
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	5	0.33
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	5	0.33
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	5	0.33
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	5	0.33
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	5	0.33
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	5	0.33
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	5	0.33
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	5	0.33
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	4	0.33
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	4	0.33
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	4	0.33
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	4	0.33
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	4	0.33
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	4	0.33
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	1	0.33
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	1	0.33
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	3	0.33
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	3	0.33
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	15	0.33
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	15	0.33
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	15	0.33
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	15	0.33
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	15	0.33
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	15	0.33
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	1	0.33
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	1	0.33
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	1	0.33
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	1	0.33
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	1	0.33
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	1	0.33
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	1	0.33
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	1	0.33
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	1	0.33
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	8	0.33
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	8	0.33
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	8	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	8	0.33
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	8	0.33
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	8	0.33
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	8	0.33
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	8	0.33
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	8	0.33
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	4	0.33
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	4	0.33
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	4	0.33
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	4	0.33
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	4	0.33
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	4	0.33
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	4	0.33
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	4	0.33
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	4	0.33
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	4	0.33
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	4	0.33
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	2	0.33
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	2	0.33
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	2	0.33
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	2	0.33
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	2	0.33
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	2	0.33
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	8	0.33
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	8	0.33
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	8	0.33
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	8	0.33
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	8	0.33
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	8	0.33
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	14	0.33
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	6	0.33
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	13	0.33
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	1	0.33
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	3	0.33
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	7	0.33
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	1	0.33
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	4	0.33
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	13	0.33
(1,262)	1:106:A:PHE:H	1:105:A:PHE:H	7	0.33
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	6	0.33
(1,115)	1:57:A:PHE:H	1:56:A:PHE:HA	13	0.33
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	14	0.33
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	14	0.33
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	14	0.33
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	14	0.33
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	14	0.33
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	14	0.33
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	14	0.33
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	14	0.33
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	14	0.33
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	7	0.32
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	7	0.32
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	7	0.32
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	2	0.32
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	2	0.32
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	13	0.32
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	13	0.32
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	7	0.32
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	7	0.32
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	10	0.32
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	10	0.32
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	10	0.32
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	13	0.32
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	13	0.32
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	13	0.32
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	13	0.32
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	13	0.32
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	13	0.32
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	13	0.32
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	13	0.32
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	13	0.32
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	14	0.32
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	14	0.32
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	14	0.32
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	14	0.32
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	14	0.32
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	14	0.32
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	14	0.32
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	14	0.32
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	14	0.32
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	14	0.32
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	14	0.32
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	13	0.32
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	13	0.32
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	13	0.32
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	13	0.32
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	13	0.32
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	13	0.32
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	13	0.32
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	13	0.32
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	10	0.32
(1,495)	1:175:A:ILE:HG21	1:172:A:THR:HA	10	0.32
(1,495)	1:175:A:ILE:HG22	1:172:A:THR:HA	10	0.32
(1,495)	1:175:A:ILE:HG23	1:172:A:THR:HA	10	0.32
(1,495)	1:175:A:ILE:HG21	1:172:A:THR:HA	15	0.32
(1,495)	1:175:A:ILE:HG22	1:172:A:THR:HA	15	0.32
(1,495)	1:175:A:ILE:HG23	1:172:A:THR:HA	15	0.32
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	7	0.32
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	3	0.32
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	3	0.32
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	8	0.32
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	2	0.32
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	5	0.32
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	15	0.32
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	15	0.32
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	15	0.32
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	15	0.32
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	3	0.32
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	5	0.32
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	15	0.32
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	3	0.32
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	3	0.32
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	15	0.32
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	15	0.32
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	15	0.32
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	5	0.32
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	2	0.32
(1,115)	1:57:A:PHE:H	1:56:A:PHE:HA	2	0.32
(1,115)	1:57:A:PHE:H	1:56:A:PHE:HA	6	0.32
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	5	0.32
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	5	0.32
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	5	0.32
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	10	0.32
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	9	0.31
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	9	0.31
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	9	0.31
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	9	0.31
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	9	0.31
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	9	0.31
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	10	0.31
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	10	0.31
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	10	0.31
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	10	0.31
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	10	0.31
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	10	0.31
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA2	6	0.31
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA3	6	0.31
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	8	0.31
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	8	0.31
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	15	0.31
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	15	0.31
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	13	0.31
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	13	0.31
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	13	0.31
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	13	0.31
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	13	0.31
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	13	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	3	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	3	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	3	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	3	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	3	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	3	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	3	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	3	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	3	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	10	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	10	0.31
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	10	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	10	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	10	0.31
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	10	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	10	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	10	0.31
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	6	0.31
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	6	0.31
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	6	0.31
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	6	0.31
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	6	0.31
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	6	0.31
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	15	0.31
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	15	0.31
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	15	0.31
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	15	0.31
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	15	0.31
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	15	0.31
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	15	0.31
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	15	0.31
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	15	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	3	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	3	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	3	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	3	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	3	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	3	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	3	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	3	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	3	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	10	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	10	0.31
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	10	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	10	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	10	0.31
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	10	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	10	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	10	0.31
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	10	0.31
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	3	0.31
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	3	0.31
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	12	0.31
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	5	0.31
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	4	0.31
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	14	0.31
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	14	0.31
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	14	0.31
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	13	0.31
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	9	0.31
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	9	0.31
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	9	0.31
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	10	0.31
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	10	0.31
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	10	0.31
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	7	0.31
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	9	0.31
(1,280)	1:111:A:LEU:H	1:111:A:LEU:HB3	14	0.31
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	4	0.31
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	14	0.31
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	12	0.31
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	4	0.31
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	4	0.31
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	4	0.31
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	10	0.31
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	10	0.31
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	10	0.31
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	12	0.31
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	4	0.31
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	5	0.3
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	5	0.3
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	5	0.3
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	5	0.3
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	5	0.3
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	5	0.3
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	6	0.3
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	6	0.3
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	6	0.3
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	6	0.3
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	6	0.3
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	6	0.3
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	8	0.3
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	8	0.3
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	8	0.3
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	8	0.3
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	8	0.3
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	8	0.3
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	11	0.3
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	11	0.3
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	14	0.3
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	6	0.3
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	6	0.3
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	6	0.3
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	6	0.3
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	6	0.3
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	6	0.3
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	6	0.3
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	6	0.3
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	6	0.3
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	4	0.3
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	5	0.3
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	6	0.3
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	6	0.3
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	6	0.3
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	6	0.3
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	6	0.3
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	6	0.3
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	11	0.3
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	11	0.3
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	5	0.3
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	5	0.3
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	5	0.3
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	5	0.3
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	5	0.3
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	5	0.3
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	8	0.3
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	8	0.3
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	8	0.3
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	8	0.3
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	8	0.3
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	8	0.3
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	12	0.3
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	12	0.3
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	6	0.3
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	6	0.3
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	6	0.3
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	6	0.3
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	6	0.3
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	6	0.3
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	6	0.3
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	6	0.3
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD11	8	0.3
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD12	8	0.3
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD13	8	0.3
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD21	8	0.3
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD22	8	0.3
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD23	8	0.3
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD11	8	0.3
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD12	8	0.3
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD13	8	0.3
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD21	8	0.3
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD22	8	0.3
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD23	8	0.3
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD11	8	0.3
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD12	8	0.3
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD13	8	0.3
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD21	8	0.3
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD22	8	0.3
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD23	8	0.3
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	7	0.3
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	6	0.3
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	11	0.3
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	5	0.3
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	5	0.3
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	3	0.3
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	11	0.3
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	2	0.3
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	3	0.3
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	4	0.3
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	8	0.3
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	10	0.3
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	12	0.3
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	14	0.3
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG21	9	0.3
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG22	9	0.3
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG23	9	0.3
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	4	0.3
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	4	0.3
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	4	0.3
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	10	0.3
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	10	0.3
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	15	0.3
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB1	7	0.3
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB2	7	0.3
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB3	7	0.3
(1,107)	1:50:A:GLY:H	1:51:A:TYR:H	11	0.3
(1,85)	1:42:A:LEU:H	1:39:A:VAL:HA	5	0.3
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	11	0.3
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	14	0.3
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	14	0.3
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	14	0.3
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	2	0.3
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	3	0.3
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	13	0.3
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	6	0.3
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	14	0.29
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	14	0.29
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	14	0.29
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	15	0.29
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	15	0.29
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	15	0.29
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE1	4	0.29
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE2	4	0.29
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE1	4	0.29
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE2	4	0.29
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE1	4	0.29
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE2	4	0.29
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	4	0.29
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	4	0.29
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	12	0.29
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	12	0.29
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	13	0.29
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	13	0.29
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	10	0.29
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	10	0.29
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	10	0.29
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD11	13	0.29
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD12	13	0.29
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD13	13	0.29
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD11	13	0.29
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD12	13	0.29
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD13	13	0.29
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD11	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD12	13	0.29
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD13	13	0.29
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	11	0.29
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	11	0.29
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	11	0.29
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	11	0.29
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	11	0.29
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	11	0.29
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	11	0.29
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	11	0.29
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	11	0.29
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	13	0.29
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	13	0.29
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	10	0.29
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	10	0.29
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	10	0.29
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	10	0.29
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	10	0.29
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	10	0.29
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	10	0.29
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	10	0.29
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	10	0.29
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	7	0.29
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	7	0.29
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	8	0.29
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	8	0.29
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	11	0.29
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	11	0.29
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	11	0.29
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	11	0.29
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	11	0.29
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	11	0.29
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	11	0.29
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	11	0.29
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	11	0.29
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	10	0.29
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	10	0.29
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	10	0.29
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	10	0.29
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	10	0.29
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	10	0.29
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	10	0.29
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	10	0.29
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	8	0.29
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	8	0.29
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	8	0.29
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	8	0.29
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	8	0.29
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	8	0.29
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	8	0.29
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	8	0.29
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	8	0.29
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	13	0.29
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	13	0.29
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	1	0.29
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	1	0.29
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	3	0.29
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	6	0.29
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	6	0.29
(1,462)	1:168:A:ILE:H	1:165:A:PHE:HA	1	0.29
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	4	0.29
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	5	0.29
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	4	0.29
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	13	0.29
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	13	0.29
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	13	0.29
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	14	0.29
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	13	0.29
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	6	0.29
(1,115)	1:57:A:PHE:H	1:56:A:PHE:HA	1	0.29
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	2	0.29
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	6	0.29
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	6	0.29
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	6	0.29
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	14	0.29
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	14	0.29
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	14	0.29
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	13	0.28
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	13	0.28
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	13	0.28
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	7	0.28
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	7	0.28
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	3	0.28
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	3	0.28
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	3	0.28
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	3	0.28
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	3	0.28
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	9	0.28
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	9	0.28
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	9	0.28
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	9	0.28
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	9	0.28
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	9	0.28
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	15	0.28
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	15	0.28
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD11	12	0.28
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD12	12	0.28
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD13	12	0.28
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD11	12	0.28
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD12	12	0.28
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD13	12	0.28
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD11	12	0.28
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD12	12	0.28
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD13	12	0.28
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	7	0.28
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	7	0.28
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	7	0.28
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	7	0.28
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	7	0.28
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	7	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	1	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	1	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	1	0.28
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	1	0.28
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	1	0.28
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	1	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	1	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	1	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	1	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	12	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	12	0.28
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	12	0.28
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	12	0.28
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	12	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	12	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	12	0.28
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	12	0.28
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	9	0.28
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	10	0.28
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	4	0.28
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	9	0.28
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	14	0.28
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	1	0.28
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	2	0.28
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	1	0.28
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	3	0.28
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	3	0.28
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	3	0.28
(1,293)	1:113:A:PHE:H	1:113:A:PHE:HB3	6	0.28
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	7	0.28
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG21	6	0.28
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG22	6	0.28
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG23	6	0.28
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	11	0.28
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	11	0.28
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	9	0.28
(1,118)	1:57:A:PHE:H	1:57:A:PHE:HB3	11	0.28
(1,115)	1:57:A:PHE:H	1:56:A:PHE:HA	3	0.28
(1,112)	1:56:A:PHE:H	1:56:A:PHE:HB3	12	0.28
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	9	0.28
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	14	0.28
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	2	0.28
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	7	0.28
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	8	0.28
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	15	0.28
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	9	0.27
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	9	0.27
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	9	0.27
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	1	0.27
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	1	0.27
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	1	0.27
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	1	0.27
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	1	0.27
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	1	0.27
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE1	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE2	15	0.27
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE1	15	0.27
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE2	15	0.27
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE1	15	0.27
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE2	15	0.27
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	5	0.27
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	5	0.27
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	5	0.27
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	5	0.27
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	5	0.27
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	5	0.27
(1,563)	1:66:A:LEU:HD11	1:113:A:PHE:HD1	13	0.27
(1,563)	1:66:A:LEU:HD11	1:113:A:PHE:HD2	13	0.27
(1,563)	1:66:A:LEU:HD12	1:113:A:PHE:HD1	13	0.27
(1,563)	1:66:A:LEU:HD12	1:113:A:PHE:HD2	13	0.27
(1,563)	1:66:A:LEU:HD13	1:113:A:PHE:HD1	13	0.27
(1,563)	1:66:A:LEU:HD13	1:113:A:PHE:HD2	13	0.27
(1,563)	1:66:A:LEU:HD21	1:113:A:PHE:HD1	13	0.27
(1,563)	1:66:A:LEU:HD21	1:113:A:PHE:HD2	13	0.27
(1,563)	1:66:A:LEU:HD22	1:113:A:PHE:HD1	13	0.27
(1,563)	1:66:A:LEU:HD22	1:113:A:PHE:HD2	13	0.27
(1,563)	1:66:A:LEU:HD23	1:113:A:PHE:HD1	13	0.27
(1,563)	1:66:A:LEU:HD23	1:113:A:PHE:HD2	13	0.27
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	14	0.27
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	14	0.27
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	14	0.27
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	14	0.27
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	14	0.27
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	14	0.27
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	14	0.27
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	14	0.27
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	14	0.27
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	6	0.27
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	6	0.27
(1,541)	1:38:A:ILE:HD11	1:67:A:PHE:HE1	15	0.27
(1,541)	1:38:A:ILE:HD11	1:67:A:PHE:HE2	15	0.27
(1,541)	1:38:A:ILE:HD12	1:67:A:PHE:HE1	15	0.27
(1,541)	1:38:A:ILE:HD12	1:67:A:PHE:HE2	15	0.27
(1,541)	1:38:A:ILE:HD13	1:67:A:PHE:HE1	15	0.27
(1,541)	1:38:A:ILE:HD13	1:67:A:PHE:HE2	15	0.27
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	10	0.27
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	10	0.27
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	10	0.27
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	10	0.27
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	10	0.27
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	10	0.27
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	10	0.27
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	10	0.27
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	9	0.27
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	9	0.27
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	15	0.27
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	8	0.27
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD21	14	0.27
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD22	14	0.27
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD21	14	0.27
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD22	14	0.27
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD21	14	0.27
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD22	14	0.27
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD21	14	0.27
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD22	14	0.27
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD21	14	0.27
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD22	14	0.27
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD21	14	0.27
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD22	14	0.27
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	13	0.27
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	9	0.27
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	5	0.27
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	7	0.27
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	13	0.27
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	10	0.27
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	13	0.27
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	10	0.27
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	10	0.27
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	10	0.27
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	10	0.27
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	1	0.27
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	3	0.27
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	5	0.27
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	11	0.27
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	12	0.27
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	9	0.26
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	9	0.26
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	8	0.26
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	14	0.26
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	14	0.26
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	14	0.26
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	14	0.26
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	14	0.26
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	14	0.26
(1,576)	1:110:A:LEU:HD21	1:105:A:PHE:HD1	4	0.26
(1,576)	1:110:A:LEU:HD21	1:105:A:PHE:HD2	4	0.26
(1,576)	1:110:A:LEU:HD22	1:105:A:PHE:HD1	4	0.26
(1,576)	1:110:A:LEU:HD22	1:105:A:PHE:HD2	4	0.26
(1,576)	1:110:A:LEU:HD23	1:105:A:PHE:HD1	4	0.26
(1,576)	1:110:A:LEU:HD23	1:105:A:PHE:HD2	4	0.26
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	2	0.26
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	2	0.26
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	2	0.26
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	2	0.26
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	2	0.26
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	2	0.26
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	9	0.26
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	9	0.26
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	9	0.26
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	9	0.26
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	9	0.26
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	9	0.26
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	1	0.26
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	1	0.26
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	1	0.26
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	1	0.26
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	1	0.26
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	1	0.26
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	12	0.26
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	12	0.26
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	15	0.26
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	8	0.26
(1,448)	1:164:A:ASN:H	1:163:A:ALA:H	13	0.26
(1,447)	1:163:A:ALA:H	1:164:A:ASN:H	13	0.26
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	12	0.26
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	12	0.26
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	5	0.26
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	5	0.26
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	5	0.26
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	5	0.26
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	5	0.26
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	10	0.26
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	10	0.26
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	10	0.26
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	10	0.26
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	10	0.26
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	10	0.26
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	9	0.26
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE21	7	0.26
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE22	7	0.26
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE21	7	0.26
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE22	7	0.26
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE21	7	0.26
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE22	7	0.26
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	2	0.26
(1,260)	1:105:A:PHE:H	1:105:A:PHE:HB3	4	0.26
(1,243)	1:91:A:MET:H	1:88:A:ALA:HA	6	0.26
(1,209)	1:84:A:VAL:HG11	1:82:A:GLU:H	14	0.26
(1,209)	1:84:A:VAL:HG12	1:82:A:GLU:H	14	0.26
(1,209)	1:84:A:VAL:HG13	1:82:A:GLU:H	14	0.26
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	2	0.26
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	11	0.26
(1,198)	1:81:A:ASP:H	1:80:A:LEU:HA	10	0.26
(1,194)	1:79:A:GLU:H	1:78:A:ASP:HA	5	0.26
(1,194)	1:79:A:GLU:H	1:78:A:ASP:HA	8	0.26
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	5	0.26
(1,101)	1:49:A:LEU:H	1:49:A:LEU:HB3	6	0.26
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	8	0.26
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	10	0.26
(1,33)	1:12:A:VAL:H	1:11:A:SER:HA	13	0.26
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	10	0.25
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	10	0.25
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	10	0.25
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	7	0.25
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	7	0.25
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	7	0.25
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	7	0.25
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	7	0.25
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	7	0.25
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	8	0.25
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	8	0.25
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	8	0.25
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	8	0.25
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	8	0.25
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	12	0.25
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	12	0.25
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	9	0.25
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	9	0.25
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	9	0.25
(1,566)	1:69:A:LEU:HD11	1:113:A:PHE:HD1	11	0.25
(1,566)	1:69:A:LEU:HD11	1:113:A:PHE:HD2	11	0.25
(1,566)	1:69:A:LEU:HD12	1:113:A:PHE:HD1	11	0.25
(1,566)	1:69:A:LEU:HD12	1:113:A:PHE:HD2	11	0.25
(1,566)	1:69:A:LEU:HD13	1:113:A:PHE:HD1	11	0.25
(1,566)	1:69:A:LEU:HD13	1:113:A:PHE:HD2	11	0.25
(1,566)	1:69:A:LEU:HD21	1:113:A:PHE:HD1	11	0.25
(1,566)	1:69:A:LEU:HD21	1:113:A:PHE:HD2	11	0.25
(1,566)	1:69:A:LEU:HD22	1:113:A:PHE:HD1	11	0.25
(1,566)	1:69:A:LEU:HD22	1:113:A:PHE:HD2	11	0.25
(1,566)	1:69:A:LEU:HD23	1:113:A:PHE:HD1	11	0.25
(1,566)	1:69:A:LEU:HD23	1:113:A:PHE:HD2	11	0.25
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD11	7	0.25
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD12	7	0.25
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD13	7	0.25
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD11	7	0.25
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD12	7	0.25
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD13	7	0.25
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD11	7	0.25
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD12	7	0.25
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD13	7	0.25
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD2	6	0.25
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD3	6	0.25
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD2	6	0.25
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD3	6	0.25
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD2	6	0.25
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD3	6	0.25
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	12	0.25
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	12	0.25
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	12	0.25
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	12	0.25
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	12	0.25
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	13	0.25
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	13	0.25
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	13	0.25
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	13	0.25
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	13	0.25
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	13	0.25
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	13	0.25
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	13	0.25
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	13	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	3	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	3	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	4	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	4	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	10	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	10	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	12	0.25
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	12	0.25
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	5	0.25
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	5	0.25
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	9	0.25
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	2	0.25
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	8	0.25
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB2	11	0.25
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB3	11	0.25
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB2	11	0.25
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB3	11	0.25
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB2	11	0.25
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB3	11	0.25
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	10	0.25
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	12	0.25
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	7	0.25
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	7	0.25
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	2	0.25
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	2	0.25
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	12	0.25
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	12	0.25
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	12	0.25
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	11	0.25
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	4	0.25
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	7	0.25
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	12	0.25
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	12	0.25
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	5	0.25
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	14	0.25
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	4	0.24
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	4	0.24
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	4	0.24
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	6	0.24
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	6	0.24
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	6	0.24
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	12	0.24
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	12	0.24
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	12	0.24
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	12	0.24
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	12	0.24
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	12	0.24
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	13	0.24
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	13	0.24
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	13	0.24
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	13	0.24
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	13	0.24
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	13	0.24
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	8	0.24
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	8	0.24
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	1	0.24
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	1	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD11	4	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD12	4	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD13	4	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD11	4	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD12	4	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD13	4	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD11	4	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD12	4	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD13	4	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD11	11	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD12	11	0.24
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD13	11	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD11	11	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD12	11	0.24
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD13	11	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD11	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD12	11	0.24
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD13	11	0.24
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	9	0.24
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	9	0.24
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	9	0.24
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	9	0.24
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	9	0.24
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	9	0.24
(1,589)	1:118:A:ALA:HB1	1:175:A:ILE:HA	3	0.24
(1,589)	1:118:A:ALA:HB2	1:175:A:ILE:HA	3	0.24
(1,589)	1:118:A:ALA:HB3	1:175:A:ILE:HA	3	0.24
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	9	0.24
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	9	0.24
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	9	0.24
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	9	0.24
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	9	0.24
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	9	0.24
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	9	0.24
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	9	0.24
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	9	0.24
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	4	0.24
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	4	0.24
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	4	0.24
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	4	0.24
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	4	0.24
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	4	0.24
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	8	0.24
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	8	0.24
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	8	0.24
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	8	0.24
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	8	0.24
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	8	0.24
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	12	0.24
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	12	0.24
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	12	0.24
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	12	0.24
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	12	0.24
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	12	0.24
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	14	0.24
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	14	0.24
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	14	0.24
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	14	0.24
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	14	0.24
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	1	0.24
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	1	0.24
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	1	0.24
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	1	0.24
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	1	0.24
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	1	0.24
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	3	0.24
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	3	0.24
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	3	0.24
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	3	0.24
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	3	0.24
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	3	0.24
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD11	9	0.24
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD12	9	0.24
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD13	9	0.24
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD11	9	0.24
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD12	9	0.24
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD13	9	0.24
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD11	9	0.24
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD12	9	0.24
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD13	9	0.24
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	1	0.24
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	1	0.24
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	1	0.24
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	1	0.24
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	1	0.24
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	1	0.24
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	9	0.24
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	9	0.24
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	9	0.24
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	9	0.24
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	9	0.24
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	9	0.24
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	9	0.24
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	9	0.24
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	9	0.24
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE2	2	0.24
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE3	2	0.24
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE2	2	0.24
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE3	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE2	2	0.24
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE3	2	0.24
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	7	0.24
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	7	0.24
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	7	0.24
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	7	0.24
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	7	0.24
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	7	0.24
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	7	0.24
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	7	0.24
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	7	0.24
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	2	0.24
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	2	0.24
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	13	0.24
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	13	0.24
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	14	0.24
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	11	0.24
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	2	0.24
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	11	0.24
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	2	0.24
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	4	0.24
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	11	0.24
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	15	0.24
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	15	0.24
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	15	0.24
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	15	0.24
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	15	0.24
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	15	0.24
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	8	0.24
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	4	0.24
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	6	0.24
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	5	0.24
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	5	0.24
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	5	0.24
(1,309)	1:118:A:ALA:HB1	1:115:A:TRP:HA	10	0.24
(1,309)	1:118:A:ALA:HB2	1:115:A:TRP:HA	10	0.24
(1,309)	1:118:A:ALA:HB3	1:115:A:TRP:HA	10	0.24
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	2	0.24
(1,281)	1:111:A:LEU:H	1:111:A:LEU:HB2	3	0.24
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	9	0.24
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	4	0.24
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:57:A:PHE:H	1:57:A:PHE:HB2	9	0.24
(1,116)	1:57:A:PHE:H	1:56:A:PHE:H	6	0.24
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	3	0.24
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	15	0.24
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	4	0.23
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	4	0.23
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	4	0.23
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	4	0.23
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	4	0.23
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	4	0.23
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	4	0.23
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	4	0.23
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	4	0.23
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	4	0.23
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	4	0.23
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	4	0.23
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	11	0.23
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	11	0.23
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	11	0.23
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	11	0.23
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	11	0.23
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	11	0.23
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	2	0.23
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	2	0.23
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	2	0.23
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	2	0.23
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	2	0.23
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	2	0.23
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	5	0.23
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	5	0.23
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	5	0.23
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	7	0.23
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	7	0.23
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	7	0.23
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	9	0.23
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	9	0.23
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	9	0.23
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	9	0.23
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	9	0.23
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	9	0.23
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	13	0.23
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	9	0.23
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	9	0.23
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	2	0.23
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	2	0.23
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	2	0.23
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	2	0.23
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	2	0.23
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	2	0.23
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	2	0.23
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	2	0.23
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	2	0.23
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	13	0.23
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	5	0.23
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	13	0.23
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	15	0.23
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	3	0.23
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	3	0.23
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	3	0.23
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	3	0.23
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	3	0.23
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	3	0.23
(1,419)	1:152:A:ALA:H	1:150:A:ILE:H	14	0.23
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	2	0.23
(1,243)	1:91:A:MET:H	1:88:A:ALA:HA	10	0.23
(1,210)	1:84:A:VAL:HG21	1:80:A:LEU:HA	8	0.23
(1,210)	1:84:A:VAL:HG22	1:80:A:LEU:HA	8	0.23
(1,210)	1:84:A:VAL:HG23	1:80:A:LEU:HA	8	0.23
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	1	0.23
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	1	0.23
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	1	0.23
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	7	0.23
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	14	0.23
(1,76)	1:39:A:VAL:H	1:40:A:ALA:H	1	0.23
(1,73)	1:39:A:VAL:H	1:36:A:PHE:HA	14	0.23
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	5	0.23
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	5	0.23
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	5	0.23
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	8	0.23
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	8	0.23
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	8	0.23
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	4	0.22
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	4	0.22
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	4	0.22
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	4	0.22
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	4	0.22
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	3	0.22
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	3	0.22
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	3	0.22
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	12	0.22
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	12	0.22
(1,609)	1:167:A:LEU:HD11	1:160:A:PHE:HD1	14	0.22
(1,609)	1:167:A:LEU:HD11	1:160:A:PHE:HD2	14	0.22
(1,609)	1:167:A:LEU:HD12	1:160:A:PHE:HD1	14	0.22
(1,609)	1:167:A:LEU:HD12	1:160:A:PHE:HD2	14	0.22
(1,609)	1:167:A:LEU:HD13	1:160:A:PHE:HD1	14	0.22
(1,609)	1:167:A:LEU:HD13	1:160:A:PHE:HD2	14	0.22
(1,609)	1:167:A:LEU:HD21	1:160:A:PHE:HD1	14	0.22
(1,609)	1:167:A:LEU:HD21	1:160:A:PHE:HD2	14	0.22
(1,609)	1:167:A:LEU:HD22	1:160:A:PHE:HD1	14	0.22
(1,609)	1:167:A:LEU:HD22	1:160:A:PHE:HD2	14	0.22
(1,609)	1:167:A:LEU:HD23	1:160:A:PHE:HD1	14	0.22
(1,609)	1:167:A:LEU:HD23	1:160:A:PHE:HD2	14	0.22
(1,607)	1:161:A:VAL:HG11	1:152:A:ALA:HA	12	0.22
(1,607)	1:161:A:VAL:HG12	1:152:A:ALA:HA	12	0.22
(1,607)	1:161:A:VAL:HG13	1:152:A:ALA:HA	12	0.22
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	1	0.22
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	1	0.22
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	1	0.22
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	1	0.22
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	1	0.22
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	1	0.22
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB2	6	0.22
(1,601)	1:150:A:ILE:H	1:170:A:LYS:HB3	6	0.22
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	14	0.22
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	14	0.22
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	14	0.22
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	14	0.22
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	14	0.22
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	14	0.22
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	14	0.22
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	14	0.22
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	14	0.22
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	8	0.22
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	8	0.22
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	13	0.22
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	13	0.22
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	13	0.22
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	13	0.22
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	13	0.22
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	13	0.22
(1,573)	1:88:A:ALA:HB1	1:76:A:LEU:HG	5	0.22
(1,573)	1:88:A:ALA:HB2	1:76:A:LEU:HG	5	0.22
(1,573)	1:88:A:ALA:HB3	1:76:A:LEU:HG	5	0.22
(1,573)	1:88:A:ALA:HB1	1:76:A:LEU:HG	11	0.22
(1,573)	1:88:A:ALA:HB2	1:76:A:LEU:HG	11	0.22
(1,573)	1:88:A:ALA:HB3	1:76:A:LEU:HG	11	0.22
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE1	4	0.22
(1,557)	1:49:A:LEU:H	1:182:A:TYR:HE2	4	0.22
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	4	0.22
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	4	0.22
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	4	0.22
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	4	0.22
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	4	0.22
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	4	0.22
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	4	0.22
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	4	0.22
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	4	0.22
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	1	0.22
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	1	0.22
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	14	0.22
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	14	0.22
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	14	0.22
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	14	0.22
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	14	0.22
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	14	0.22
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	14	0.22
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	14	0.22
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	14	0.22
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	5	0.22
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	5	0.22
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	10	0.22
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	2	0.22
(1,490)	1:174:A:ALA:H	1:171:A:VAL:HA	15	0.22
(1,485)	1:172:A:THR:H	1:174:A:ALA:H	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	14	0.22
(1,371)	1:140:A:LEU:H	1:137:A:LEU:H	8	0.22
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	6	0.22
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	9	0.22
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	11	0.22
(1,296)	1:114:A:LEU:H	1:111:A:LEU:HA	2	0.22
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	1	0.22
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	6	0.22
(1,73)	1:39:A:VAL:H	1:36:A:PHE:HA	11	0.22
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	11	0.22
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	11	0.22
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	11	0.22
(1,28)	1:11:A:SER:H	1:8:A:GLY:HA2	8	0.22
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	3	0.22
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE1	13	0.21
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE2	13	0.21
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE1	13	0.21
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE2	13	0.21
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE1	13	0.21
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE2	13	0.21
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA2	9	0.21
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA3	9	0.21
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	14	0.21
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	14	0.21
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	14	0.21
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	4	0.21
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	4	0.21
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	4	0.21
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	3	0.21
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	3	0.21
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	3	0.21
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	3	0.21
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	3	0.21
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	3	0.21
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD1	15	0.21
(1,548)	1:42:A:LEU:HD11	1:182:A:TYR:HD2	15	0.21
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD1	15	0.21
(1,548)	1:42:A:LEU:HD12	1:182:A:TYR:HD2	15	0.21
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD1	15	0.21
(1,548)	1:42:A:LEU:HD13	1:182:A:TYR:HD2	15	0.21
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	5	0.21
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD2	1	0.21
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD3	1	0.21
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD2	1	0.21
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD3	1	0.21
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD2	1	0.21
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD3	1	0.21
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	1	0.21
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	1	0.21
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	7	0.21
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	7	0.21
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	14	0.21
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	14	0.21
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	5	0.21
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	5	0.21
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	8	0.21
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	8	0.21
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	6	0.21
(1,327)	1:125:A:ILE:HD11	1:122:A:PHE:HD1	13	0.21
(1,327)	1:125:A:ILE:HD11	1:122:A:PHE:HD2	13	0.21
(1,327)	1:125:A:ILE:HD12	1:122:A:PHE:HD1	13	0.21
(1,327)	1:125:A:ILE:HD12	1:122:A:PHE:HD2	13	0.21
(1,327)	1:125:A:ILE:HD13	1:122:A:PHE:HD1	13	0.21
(1,327)	1:125:A:ILE:HD13	1:122:A:PHE:HD2	13	0.21
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	8	0.21
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	8	0.21
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	8	0.21
(1,299)	1:114:A:LEU:H	1:114:A:LEU:HB3	4	0.21
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	15	0.21
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	9	0.21
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	12	0.21
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	3	0.21
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	3	0.21
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	2	0.21
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	3	0.21
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	3	0.21
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	3	0.21
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB1	3	0.21
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB2	3	0.21
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB3	3	0.21
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB1	4	0.21
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB2	4	0.21
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	4	0.21
(1,32)	1:12:A:VAL:H	1:9:A:ILE:HA	9	0.21
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	11	0.21
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	11	0.21
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	11	0.21
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	11	0.21
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	11	0.21
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	11	0.21
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	11	0.21
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	11	0.21
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	11	0.21
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	3	0.2
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	3	0.2
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	3	0.2
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	3	0.2
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	3	0.2
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	3	0.2
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	4	0.2
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	4	0.2
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	4	0.2
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	4	0.2
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	4	0.2
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	4	0.2
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	1	0.2
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	1	0.2
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	4	0.2
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	4	0.2
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	9	0.2
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	9	0.2
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	11	0.2
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	11	0.2
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	11	0.2
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	11	0.2
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	11	0.2
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	11	0.2
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	2	0.2
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	2	0.2
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	2	0.2
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	2	0.2
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	2	0.2
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	2	0.2
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	13	0.2
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	13	0.2
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	15	0.2
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	15	0.2
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	15	0.2
(1,574)	1:90:A:ARG:H	1:115:A:TRP:HZ2	7	0.2
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	8	0.2
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	8	0.2
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	8	0.2
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	8	0.2
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	8	0.2
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	8	0.2
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	6	0.2
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	6	0.2
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	6	0.2
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	6	0.2
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	6	0.2
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	6	0.2
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	6	0.2
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	6	0.2
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	6	0.2
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	2	0.2
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	2	0.2
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	7	0.2
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	7	0.2
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	15	0.2
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	15	0.2
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	15	0.2
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	15	0.2
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	15	0.2
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	15	0.2
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	15	0.2
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	15	0.2
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	15	0.2
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	15	0.2
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	15	0.2
(1,504)	1:178:A:LEU:HD11	1:175:A:ILE:HA	2	0.2
(1,504)	1:178:A:LEU:HD12	1:175:A:ILE:HA	2	0.2
(1,504)	1:178:A:LEU:HD13	1:175:A:ILE:HA	2	0.2
(1,504)	1:178:A:LEU:HD11	1:175:A:ILE:HA	9	0.2
(1,504)	1:178:A:LEU:HD12	1:175:A:ILE:HA	9	0.2
(1,504)	1:178:A:LEU:HD13	1:175:A:ILE:HA	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	15	0.2
(1,476)	1:171:A:VAL:H	1:168:A:ILE:HA	7	0.2
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	13	0.2
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	2	0.2
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	2	0.2
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	14	0.2
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	1	0.2
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	12	0.2
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	13	0.2
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG21	12	0.2
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG22	12	0.2
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG23	12	0.2
(1,225)	1:87:A:PHE:H	1:87:A:PHE:HB2	5	0.2
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	6	0.2
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	6	0.2
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	6	0.2
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	7	0.2
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	1	0.2
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	12	0.2
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	10	0.2
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	4	0.2
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	4	0.2
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	4	0.2
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB1	4	0.2
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB2	4	0.2
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB3	4	0.2
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	7	0.2
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	7	0.2
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	15	0.2
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	13	0.19
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	13	0.19
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	13	0.19
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	13	0.19
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	13	0.19
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	13	0.19
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	5	0.19
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	5	0.19
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	5	0.19
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	12	0.19
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	12	0.19
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	12	0.19
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	2	0.19
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	2	0.19
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	2	0.19
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	2	0.19
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	2	0.19
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	15	0.19
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	15	0.19
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	15	0.19
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	15	0.19
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	15	0.19
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	15	0.19
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE1	14	0.19
(1,618)	1:178:A:LEU:HD11	1:122:A:PHE:HE2	14	0.19
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE1	14	0.19
(1,618)	1:178:A:LEU:HD12	1:122:A:PHE:HE2	14	0.19
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE1	14	0.19
(1,618)	1:178:A:LEU:HD13	1:122:A:PHE:HE2	14	0.19
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA2	13	0.19
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA3	13	0.19
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	10	0.19
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	10	0.19
(1,607)	1:161:A:VAL:HG11	1:152:A:ALA:HA	1	0.19
(1,607)	1:161:A:VAL:HG12	1:152:A:ALA:HA	1	0.19
(1,607)	1:161:A:VAL:HG13	1:152:A:ALA:HA	1	0.19
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	10	0.19
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	10	0.19
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	10	0.19
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	10	0.19
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	10	0.19
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	10	0.19
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE2	6	0.19
(1,602)	1:150:A:ILE:HG21	1:170:A:LYS:HE3	6	0.19
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE2	6	0.19
(1,602)	1:150:A:ILE:HG22	1:170:A:LYS:HE3	6	0.19
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE2	6	0.19
(1,602)	1:150:A:ILE:HG23	1:170:A:LYS:HE3	6	0.19
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	9	0.19
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	9	0.19
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	9	0.19
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	12	0.19
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	12	0.19
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	12	0.19
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	12	0.19
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	12	0.19
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	12	0.19
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	12	0.19
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	12	0.19
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	11	0.19
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	11	0.19
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	11	0.19
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	2	0.19
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	2	0.19
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	13	0.19
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	13	0.19
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	13	0.19
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	12	0.19
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	12	0.19
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	12	0.19
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	12	0.19
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	12	0.19
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	12	0.19
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	12	0.19
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	12	0.19
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	12	0.19
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	12	0.19
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	12	0.19
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	12	0.19
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	12	0.19
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	12	0.19
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	12	0.19
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD1	2	0.19
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD2	2	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	5	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	5	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	5	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	5	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	5	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	5	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	5	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	5	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	5	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	11	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	11	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	11	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	11	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	11	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	11	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	11	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	11	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	14	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	14	0.19
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	14	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	14	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	14	0.19
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	14	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	14	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	14	0.19
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	14	0.19
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE2	9	0.19
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE3	9	0.19
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE2	9	0.19
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE3	9	0.19
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE2	9	0.19
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE3	9	0.19
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	5	0.19
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	5	0.19
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	5	0.19
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	5	0.19
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	5	0.19
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	5	0.19
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	5	0.19
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	5	0.19
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	5	0.19
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	11	0.19
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	11	0.19
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD2	7	0.19
(1,524)	1:8:A:GLY:H	1:121:A:PRO:HD3	7	0.19
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	3	0.19
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	7	0.19
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	1	0.19
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	7	0.19
(1,495)	1:175:A:ILE:HG21	1:172:A:THR:HA	7	0.19
(1,495)	1:175:A:ILE:HG22	1:172:A:THR:HA	7	0.19
(1,495)	1:175:A:ILE:HG23	1:172:A:THR:HA	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:175:A:ILE:HG21	1:172:A:THR:HA	9	0.19
(1,495)	1:175:A:ILE:HG22	1:172:A:THR:HA	9	0.19
(1,495)	1:175:A:ILE:HG23	1:172:A:THR:HA	9	0.19
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	3	0.19
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	3	0.19
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	15	0.19
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	1	0.19
(1,327)	1:125:A:ILE:HD11	1:122:A:PHE:HD1	15	0.19
(1,327)	1:125:A:ILE:HD11	1:122:A:PHE:HD2	15	0.19
(1,327)	1:125:A:ILE:HD12	1:122:A:PHE:HD1	15	0.19
(1,327)	1:125:A:ILE:HD12	1:122:A:PHE:HD2	15	0.19
(1,327)	1:125:A:ILE:HD13	1:122:A:PHE:HD1	15	0.19
(1,327)	1:125:A:ILE:HD13	1:122:A:PHE:HD2	15	0.19
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	8	0.19
(1,289)	1:112:A:ALA:H	1:114:A:LEU:H	2	0.19
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	14	0.19
(1,206)	1:84:A:VAL:H	1:83:A:LYS:H	13	0.19
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	4	0.19
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	14	0.19
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	10	0.19
(1,119)	1:57:A:PHE:H	1:57:A:PHE:HB2	7	0.19
(1,119)	1:57:A:PHE:H	1:57:A:PHE:HB2	14	0.19
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB1	1	0.19
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB2	1	0.19
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB3	1	0.19
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	5	0.19
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	5	0.19
(1,73)	1:39:A:VAL:H	1:36:A:PHE:HA	2	0.19
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG21	12	0.19
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG22	12	0.19
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG23	12	0.19
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG21	12	0.19
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG22	12	0.19
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG23	12	0.19
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG21	12	0.19
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG22	12	0.19
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG23	12	0.19
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	15	0.19
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	15	0.19
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	15	0.19
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	10	0.18
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	6	0.18
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	6	0.18
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	6	0.18
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	5	0.18
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	5	0.18
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	5	0.18
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	5	0.18
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	5	0.18
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	5	0.18
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	1	0.18
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	1	0.18
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	1	0.18
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	1	0.18
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	1	0.18
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	1	0.18
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	1	0.18
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	1	0.18
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	1	0.18
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG11	4	0.18
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG12	4	0.18
(1,588)	1:118:A:ALA:HB1	1:39:A:VAL:HG13	4	0.18
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG11	4	0.18
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG12	4	0.18
(1,588)	1:118:A:ALA:HB2	1:39:A:VAL:HG13	4	0.18
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG11	4	0.18
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG12	4	0.18
(1,588)	1:118:A:ALA:HB3	1:39:A:VAL:HG13	4	0.18
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	10	0.18
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	10	0.18
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	10	0.18
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	10	0.18
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	10	0.18
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	10	0.18
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD2	9	0.18
(1,582)	1:115:A:TRP:H	1:90:A:ARG:HD3	9	0.18
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	2	0.18
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	2	0.18
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	2	0.18
(1,567)	1:75:A:LEU:HD11	1:81:A:ASP:HB2	12	0.18
(1,567)	1:75:A:LEU:HD11	1:81:A:ASP:HB3	12	0.18
(1,567)	1:75:A:LEU:HD12	1:81:A:ASP:HB2	12	0.18
(1,567)	1:75:A:LEU:HD12	1:81:A:ASP:HB3	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:75:A:LEU:HD13	1:81:A:ASP:HB2	12	0.18
(1,567)	1:75:A:LEU:HD13	1:81:A:ASP:HB3	12	0.18
(1,564)	1:68:A:LEU:HD11	1:117:A:PRO:HD2	11	0.18
(1,564)	1:68:A:LEU:HD11	1:117:A:PRO:HD3	11	0.18
(1,564)	1:68:A:LEU:HD12	1:117:A:PRO:HD2	11	0.18
(1,564)	1:68:A:LEU:HD12	1:117:A:PRO:HD3	11	0.18
(1,564)	1:68:A:LEU:HD13	1:117:A:PRO:HD2	11	0.18
(1,564)	1:68:A:LEU:HD13	1:117:A:PRO:HD3	11	0.18
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	10	0.18
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	10	0.18
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	10	0.18
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	10	0.18
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	10	0.18
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	10	0.18
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	5	0.18
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	5	0.18
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	5	0.18
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	5	0.18
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	5	0.18
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	5	0.18
(1,543)	1:40:A:ALA:HB1	1:4:A:ALA:HB1	11	0.18
(1,543)	1:40:A:ALA:HB1	1:4:A:ALA:HB2	11	0.18
(1,543)	1:40:A:ALA:HB1	1:4:A:ALA:HB3	11	0.18
(1,543)	1:40:A:ALA:HB2	1:4:A:ALA:HB1	11	0.18
(1,543)	1:40:A:ALA:HB2	1:4:A:ALA:HB2	11	0.18
(1,543)	1:40:A:ALA:HB2	1:4:A:ALA:HB3	11	0.18
(1,543)	1:40:A:ALA:HB3	1:4:A:ALA:HB1	11	0.18
(1,543)	1:40:A:ALA:HB3	1:4:A:ALA:HB2	11	0.18
(1,543)	1:40:A:ALA:HB3	1:4:A:ALA:HB3	11	0.18
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB1	4	0.18
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB2	4	0.18
(1,542)	1:39:A:VAL:HG11	1:118:A:ALA:HB3	4	0.18
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB1	4	0.18
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB2	4	0.18
(1,542)	1:39:A:VAL:HG12	1:118:A:ALA:HB3	4	0.18
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB1	4	0.18
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB2	4	0.18
(1,542)	1:39:A:VAL:HG13	1:118:A:ALA:HB3	4	0.18
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	2	0.18
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	2	0.18
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	2	0.18
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	2	0.18
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	2	0.18
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	15	0.18
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	15	0.18
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	1	0.18
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	3	0.18
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	6	0.18
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	12	0.18
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	3	0.18
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	14	0.18
(1,468)	1:169:A:ARG:H	1:167:A:LEU:H	13	0.18
(1,462)	1:168:A:ILE:H	1:165:A:PHE:HA	10	0.18
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	1	0.18
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	14	0.18
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	8	0.18
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	12	0.18
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	7	0.18
(1,377)	1:141:A:SER:H	1:138:A:VAL:H	8	0.18
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD1	8	0.18
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD2	8	0.18
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD1	8	0.18
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD2	8	0.18
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD1	8	0.18
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD2	8	0.18
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	10	0.18
(1,309)	1:118:A:ALA:HB1	1:115:A:TRP:HA	4	0.18
(1,309)	1:118:A:ALA:HB2	1:115:A:TRP:HA	4	0.18
(1,309)	1:118:A:ALA:HB3	1:115:A:TRP:HA	4	0.18
(1,309)	1:118:A:ALA:HB1	1:115:A:TRP:HA	5	0.18
(1,309)	1:118:A:ALA:HB2	1:115:A:TRP:HA	5	0.18
(1,309)	1:118:A:ALA:HB3	1:115:A:TRP:HA	5	0.18
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	4	0.18
(1,278)	1:111:A:LEU:H	1:108:A:GLY:HA2	11	0.18
(1,278)	1:111:A:LEU:H	1:108:A:GLY:HA3	11	0.18
(1,271)	1:109:A:MET:H	1:109:A:MET:HB3	14	0.18
(1,263)	1:106:A:PHE:H	1:107:A:PHE:H	5	0.18
(1,261)	1:105:A:PHE:H	1:105:A:PHE:HB2	4	0.18
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	9	0.18
(1,183)	1:76:A:LEU:H	1:72:A:ALA:HB1	11	0.18
(1,183)	1:76:A:LEU:H	1:72:A:ALA:HB2	11	0.18
(1,183)	1:76:A:LEU:H	1:72:A:ALA:HB3	11	0.18
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	11	0.18
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	15	0.18
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	8	0.18
(1,119)	1:57:A:PHE:H	1:57:A:PHE:HB2	12	0.18
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	8	0.18
(1,73)	1:39:A:VAL:H	1:36:A:PHE:HA	4	0.18
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	14	0.18
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	14	0.18
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	14	0.18
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	8	0.18
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	8	0.18
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	8	0.18
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	4	0.18
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	4	0.18
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	4	0.18
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	11	0.18
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	12	0.18
(1,32)	1:12:A:VAL:H	1:9:A:ILE:HA	4	0.18
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	9	0.18
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	1	0.17
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	1	0.17
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	1	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD11	3	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD12	3	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD13	3	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD11	10	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD12	10	0.17
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD13	10	0.17
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	14	0.17
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	14	0.17
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	14	0.17
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	14	0.17
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	14	0.17
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	14	0.17
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	3	0.17
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	3	0.17
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	3	0.17
(1,573)	1:88:A:ALA:HB1	1:76:A:LEU:HG	3	0.17
(1,573)	1:88:A:ALA:HB2	1:76:A:LEU:HG	3	0.17
(1,573)	1:88:A:ALA:HB3	1:76:A:LEU:HG	3	0.17
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	1	0.17
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	1	0.17
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	1	0.17
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	1	0.17
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	1	0.17
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	1	0.17
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	1	0.17
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	1	0.17
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	3	0.17
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	3	0.17
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	3	0.17
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	3	0.17
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	3	0.17
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	3	0.17
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	2	0.17
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	2	0.17
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	2	0.17
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	2	0.17
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	2	0.17
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	2	0.17
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	14	0.17
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	14	0.17
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	14	0.17
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	14	0.17
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	14	0.17
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	14	0.17
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB1	6	0.17
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB2	6	0.17
(1,532)	1:16:A:ALA:HB1	1:163:A:ALA:HB3	6	0.17
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB1	6	0.17
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB2	6	0.17
(1,532)	1:16:A:ALA:HB2	1:163:A:ALA:HB3	6	0.17
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB1	6	0.17
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB2	6	0.17
(1,532)	1:16:A:ALA:HB3	1:163:A:ALA:HB3	6	0.17
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	5	0.17
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	5	0.17
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	2	0.17
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	2	0.17
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	5	0.17
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	5	0.17
(1,476)	1:171:A:VAL:H	1:168:A:ILE:HA	13	0.17
(1,476)	1:171:A:VAL:H	1:168:A:ILE:HA	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,462)	1:168:A:ILE:H	1:165:A:PHE:HA	15	0.17
(1,446)	1:163:A:ALA:H	1:162:A:LYS:H	3	0.17
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	13	0.17
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	1	0.17
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	4	0.17
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	7	0.17
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD1	7	0.17
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD2	7	0.17
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD1	7	0.17
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD2	7	0.17
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD1	7	0.17
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD2	7	0.17
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE21	13	0.17
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE22	13	0.17
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE21	13	0.17
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE22	13	0.17
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE21	13	0.17
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE22	13	0.17
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE21	15	0.17
(1,326)	1:125:A:ILE:HG21	1:129:A:GLN:HE22	15	0.17
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE21	15	0.17
(1,326)	1:125:A:ILE:HG22	1:129:A:GLN:HE22	15	0.17
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE21	15	0.17
(1,326)	1:125:A:ILE:HG23	1:129:A:GLN:HE22	15	0.17
(1,280)	1:111:A:LEU:H	1:111:A:LEU:HB3	15	0.17
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	1	0.17
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	6	0.17
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	11	0.17
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	11	0.17
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	11	0.17
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	15	0.17
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	10	0.17
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	9	0.17
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	9	0.17
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	9	0.17
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	6	0.17
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	6	0.17
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	6	0.17
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	11	0.17
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	3	0.17
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	3	0.17
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	3	0.17
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	1	0.17
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	1	0.17
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	1	0.17
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	15	0.17
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	15	0.17
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	15	0.17
(1,43)	1:17:A:VAL:H	1:16:A:ALA:HA	4	0.17
(1,42)	1:14:A:SER:H	1:13:A:PHE:H	1	0.17
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	7	0.17
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	11	0.16
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	11	0.16
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	11	0.16
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	11	0.16
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	11	0.16
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	11	0.16
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD11	8	0.16
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD12	8	0.16
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD13	8	0.16
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	5	0.16
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	5	0.16
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	5	0.16
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE1	7	0.16
(1,586)	1:118:A:ALA:HB1	1:25:A:PHE:HE2	7	0.16
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE1	7	0.16
(1,586)	1:118:A:ALA:HB2	1:25:A:PHE:HE2	7	0.16
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE1	7	0.16
(1,586)	1:118:A:ALA:HB3	1:25:A:PHE:HE2	7	0.16
(1,576)	1:110:A:LEU:HD21	1:105:A:PHE:HD1	3	0.16
(1,576)	1:110:A:LEU:HD21	1:105:A:PHE:HD2	3	0.16
(1,576)	1:110:A:LEU:HD22	1:105:A:PHE:HD1	3	0.16
(1,576)	1:110:A:LEU:HD22	1:105:A:PHE:HD2	3	0.16
(1,576)	1:110:A:LEU:HD23	1:105:A:PHE:HD1	3	0.16
(1,576)	1:110:A:LEU:HD23	1:105:A:PHE:HD2	3	0.16
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD11	3	0.16
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD12	3	0.16
(1,562)	1:63:A:VAL:HG11	1:110:A:LEU:HD13	3	0.16
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD11	3	0.16
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD12	3	0.16
(1,562)	1:63:A:VAL:HG12	1:110:A:LEU:HD13	3	0.16
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD11	3	0.16
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD12	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:63:A:VAL:HG13	1:110:A:LEU:HD13	3	0.16
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	15	0.16
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	15	0.16
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	15	0.16
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	15	0.16
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	15	0.16
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	15	0.16
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	1	0.16
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	1	0.16
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	1	0.16
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	1	0.16
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	1	0.16
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	1	0.16
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	3	0.16
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	3	0.16
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	3	0.16
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	3	0.16
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	3	0.16
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	3	0.16
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	10	0.16
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	10	0.16
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	10	0.16
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	10	0.16
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	10	0.16
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	10	0.16
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD11	8	0.16
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD12	8	0.16
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD13	8	0.16
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD11	8	0.16
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD12	8	0.16
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD13	8	0.16
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD11	8	0.16
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD12	8	0.16
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD13	8	0.16
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD11	12	0.16
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD12	12	0.16
(1,552)	1:43:A:THR:HG21	1:178:A:LEU:HD13	12	0.16
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD11	12	0.16
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD12	12	0.16
(1,552)	1:43:A:THR:HG22	1:178:A:LEU:HD13	12	0.16
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD11	12	0.16
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD12	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:43:A:THR:HG23	1:178:A:LEU:HD13	12	0.16
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	3	0.16
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	3	0.16
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD2	15	0.16
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD3	15	0.16
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD2	15	0.16
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD3	15	0.16
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD2	15	0.16
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD3	15	0.16
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	7	0.16
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	7	0.16
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	7	0.16
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	7	0.16
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	7	0.16
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	7	0.16
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD1	6	0.16
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD2	6	0.16
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	7	0.16
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	7	0.16
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	7	0.16
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	7	0.16
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	7	0.16
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	7	0.16
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	7	0.16
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	7	0.16
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	7	0.16
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	12	0.16
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	13	0.16
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	1	0.16
(1,485)	1:172:A:THR:H	1:174:A:ALA:H	7	0.16
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	5	0.16
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD21	12	0.16
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD22	12	0.16
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD21	12	0.16
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD22	12	0.16
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD21	12	0.16
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD22	12	0.16
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD21	12	0.16
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD22	12	0.16
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD21	12	0.16
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD22	12	0.16
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD21	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD22	12	0.16
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	9	0.16
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	12	0.16
(1,423)	1:153:A:VAL:H	1:150:A:ILE:HA	7	0.16
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	10	0.16
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	9	0.16
(1,309)	1:118:A:ALA:HB1	1:115:A:TRP:HA	2	0.16
(1,309)	1:118:A:ALA:HB2	1:115:A:TRP:HA	2	0.16
(1,309)	1:118:A:ALA:HB3	1:115:A:TRP:HA	2	0.16
(1,296)	1:114:A:LEU:H	1:111:A:LEU:HA	9	0.16
(1,281)	1:111:A:LEU:H	1:111:A:LEU:HB2	4	0.16
(1,243)	1:91:A:MET:H	1:88:A:ALA:HA	4	0.16
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG21	15	0.16
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG22	15	0.16
(1,235)	1:89:A:SER:H	1:86:A:ILE:HG23	15	0.16
(1,209)	1:84:A:VAL:HG11	1:82:A:GLU:H	6	0.16
(1,209)	1:84:A:VAL:HG12	1:82:A:GLU:H	6	0.16
(1,209)	1:84:A:VAL:HG13	1:82:A:GLU:H	6	0.16
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	5	0.16
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	5	0.16
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	5	0.16
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	3	0.16
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	10	0.16
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	2	0.16
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	11	0.16
(1,116)	1:57:A:PHE:H	1:56:A:PHE:H	5	0.16
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	1	0.16
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	13	0.16
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG21	9	0.16
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG22	9	0.16
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG23	9	0.16
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG21	9	0.16
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG22	9	0.16
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG23	9	0.16
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG21	9	0.16
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG22	9	0.16
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG23	9	0.16
(1,47)	1:20:A:VAL:H	1:17:A:VAL:HB	11	0.16
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	2	0.16
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	15	0.16
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	1	0.16
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	1	0.16
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	1	0.16
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	1	0.16
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	1	0.16
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	1	0.16
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	1	0.16
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	1	0.16
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	8	0.15
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	8	0.15
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	8	0.15
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	12	0.15
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	12	0.15
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG12	6	0.15
(1,613)	1:174:A:ALA:H	1:119:A:ILE:HG13	6	0.15
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG2	6	0.15
(1,611)	1:171:A:VAL:H	1:83:A:LYS:HG3	6	0.15
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	7	0.15
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	7	0.15
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	7	0.15
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	7	0.15
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	7	0.15
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	7	0.15
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD1	8	0.15
(1,604)	1:153:A:VAL:HG21	1:160:A:PHE:HD2	8	0.15
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD1	8	0.15
(1,604)	1:153:A:VAL:HG22	1:160:A:PHE:HD2	8	0.15
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD1	8	0.15
(1,604)	1:153:A:VAL:HG23	1:160:A:PHE:HD2	8	0.15
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	7	0.15
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	7	0.15
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	7	0.15
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	11	0.15
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	11	0.15
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	11	0.15
(1,589)	1:118:A:ALA:HB1	1:175:A:ILE:HA	5	0.15
(1,589)	1:118:A:ALA:HB2	1:175:A:ILE:HA	5	0.15
(1,589)	1:118:A:ALA:HB3	1:175:A:ILE:HA	5	0.15
(1,583)	1:116:A:LEU:HD11	1:71:A:PHE:HB2	12	0.15
(1,583)	1:116:A:LEU:HD11	1:71:A:PHE:HB3	12	0.15
(1,583)	1:116:A:LEU:HD12	1:71:A:PHE:HB2	12	0.15
(1,583)	1:116:A:LEU:HD12	1:71:A:PHE:HB3	12	0.15
(1,583)	1:116:A:LEU:HD13	1:71:A:PHE:HB2	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:116:A:LEU:HD13	1:71:A:PHE:HB3	12	0.15
(1,583)	1:116:A:LEU:HD21	1:71:A:PHE:HB2	12	0.15
(1,583)	1:116:A:LEU:HD21	1:71:A:PHE:HB3	12	0.15
(1,583)	1:116:A:LEU:HD22	1:71:A:PHE:HB2	12	0.15
(1,583)	1:116:A:LEU:HD22	1:71:A:PHE:HB3	12	0.15
(1,583)	1:116:A:LEU:HD23	1:71:A:PHE:HB2	12	0.15
(1,583)	1:116:A:LEU:HD23	1:71:A:PHE:HB3	12	0.15
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	9	0.15
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	9	0.15
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	9	0.15
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	9	0.15
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	9	0.15
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	9	0.15
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	10	0.15
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	10	0.15
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	10	0.15
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	10	0.15
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	10	0.15
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	10	0.15
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB2	9	0.15
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB3	9	0.15
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	8	0.15
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	8	0.15
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	8	0.15
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	8	0.15
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	8	0.15
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	8	0.15
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	8	0.15
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	8	0.15
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	8	0.15
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	8	0.15
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	8	0.15
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	8	0.15
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB2	8	0.15
(1,546)	1:42:A:LEU:H	1:117:A:PRO:HB3	8	0.15
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB2	14	0.15
(1,545)	1:41:A:GLY:H	1:117:A:PRO:HB3	14	0.15
(1,534)	1:24:A:ILE:HD11	1:17:A:VAL:HB	14	0.15
(1,534)	1:24:A:ILE:HD12	1:17:A:VAL:HB	14	0.15
(1,534)	1:24:A:ILE:HD13	1:17:A:VAL:HB	14	0.15
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	8	0.15
(1,504)	1:178:A:LEU:HD11	1:175:A:ILE:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:178:A:LEU:HD12	1:175:A:ILE:HA	6	0.15
(1,504)	1:178:A:LEU:HD13	1:175:A:ILE:HA	6	0.15
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	10	0.15
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	8	0.15
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	12	0.15
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	10	0.15
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	10	0.15
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	7	0.15
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD1	2	0.15
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD2	2	0.15
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD1	2	0.15
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD2	2	0.15
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD1	2	0.15
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD2	2	0.15
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	11	0.15
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	11	0.15
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	11	0.15
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	10	0.15
(1,243)	1:91:A:MET:H	1:88:A:ALA:HA	2	0.15
(1,243)	1:91:A:MET:H	1:88:A:ALA:HA	9	0.15
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	8	0.15
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	8	0.15
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	8	0.15
(1,166)	1:72:A:ALA:H	1:74:A:ILE:H	2	0.15
(1,146)	1:65:A:MET:H	1:62:A:VAL:HA	9	0.15
(1,116)	1:57:A:PHE:H	1:56:A:PHE:H	1	0.15
(1,116)	1:57:A:PHE:H	1:56:A:PHE:H	3	0.15
(1,113)	1:56:A:PHE:H	1:56:A:PHE:HB2	5	0.15
(1,101)	1:49:A:LEU:H	1:49:A:LEU:HB3	10	0.15
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	7	0.15
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG21	8	0.15
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG22	8	0.15
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG23	8	0.15
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG21	8	0.15
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG22	8	0.15
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG23	8	0.15
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG21	8	0.15
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG22	8	0.15
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG23	8	0.15
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	15	0.15
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	15	0.15
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	2	0.15
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	2	0.15
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	2	0.15
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG21	8	0.15
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG22	8	0.15
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG23	8	0.15
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG21	8	0.15
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG22	8	0.15
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG23	8	0.15
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG21	8	0.15
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG22	8	0.15
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG23	8	0.15
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG21	8	0.15
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG22	8	0.15
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG23	8	0.15
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG21	8	0.15
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG22	8	0.15
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG23	8	0.15
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG21	8	0.15
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG22	8	0.15
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG23	8	0.15
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB1	15	0.15
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB2	15	0.15
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB3	15	0.15
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	12	0.15
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	2	0.15
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	2	0.15
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	2	0.15
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	2	0.15
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	2	0.15
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	2	0.15
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	2	0.15
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	2	0.15
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	2	0.15
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	6	0.14
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	6	0.14
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	6	0.14
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	6	0.14
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	6	0.14
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	6	0.14
(1,617)	1:177:A:LEU:HD11	1:122:A:PHE:HE1	15	0.14
(1,617)	1:177:A:LEU:HD11	1:122:A:PHE:HE2	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,617)	1:177:A:LEU:HD12	1:122:A:PHE:HE1	15	0.14
(1,617)	1:177:A:LEU:HD12	1:122:A:PHE:HE2	15	0.14
(1,617)	1:177:A:LEU:HD13	1:122:A:PHE:HE1	15	0.14
(1,617)	1:177:A:LEU:HD13	1:122:A:PHE:HE2	15	0.14
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	1	0.14
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	1	0.14
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	1	0.14
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	2	0.14
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	2	0.14
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	2	0.14
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	2	0.14
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	2	0.14
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	2	0.14
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	11	0.14
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	11	0.14
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	11	0.14
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	11	0.14
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	11	0.14
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	11	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	1	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	1	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	1	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	1	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	1	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	1	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	1	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	1	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	1	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	7	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	7	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	7	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	7	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	7	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	7	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	7	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	7	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	7	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	13	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	13	0.14
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	13	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	13	0.14
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	13	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	13	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	13	0.14
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	13	0.14
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	15	0.14
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	15	0.14
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	15	0.14
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	15	0.14
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	15	0.14
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	15	0.14
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD1	8	0.14
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD2	8	0.14
(1,534)	1:24:A:ILE:HD11	1:17:A:VAL:HB	11	0.14
(1,534)	1:24:A:ILE:HD12	1:17:A:VAL:HB	11	0.14
(1,534)	1:24:A:ILE:HD13	1:17:A:VAL:HB	11	0.14
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	11	0.14
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	13	0.14
(1,497)	1:176:A:VAL:H	1:172:A:THR:HA	6	0.14
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	1	0.14
(1,476)	1:171:A:VAL:H	1:168:A:ILE:HA	2	0.14
(1,472)	1:170:A:LYS:H	1:167:A:LEU:HA	11	0.14
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	7	0.14
(1,446)	1:163:A:ALA:H	1:162:A:LYS:H	1	0.14
(1,446)	1:163:A:ALA:H	1:162:A:LYS:H	7	0.14
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	5	0.14
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	11	0.14
(1,391)	1:143:A:GLY:H	1:144:A:LEU:H	1	0.14
(1,390)	1:143:A:GLY:H	1:144:A:LEU:H	1	0.14
(1,371)	1:140:A:LEU:H	1:137:A:LEU:H	10	0.14
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	15	0.14
(1,339)	1:128:A:SER:H	1:125:A:ILE:HA	3	0.14
(1,334)	1:127:A:ILE:H	1:124:A:GLY:HA2	10	0.14
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	13	0.14
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	15	0.14
(1,284)	1:112:A:ALA:H	1:109:A:MET:HA	6	0.14
(1,262)	1:106:A:PHE:H	1:105:A:PHE:H	9	0.14
(1,260)	1:105:A:PHE:H	1:105:A:PHE:HB3	7	0.14
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	4	0.14
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	4	0.14
(1,211)	1:84:A:VAL:HG21	1:81:A:ASP:HA	14	0.14
(1,211)	1:84:A:VAL:HG22	1:81:A:ASP:HA	14	0.14
(1,211)	1:84:A:VAL:HG23	1:81:A:ASP:HA	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:84:A:VAL:HG21	1:80:A:LEU:HA	11	0.14
(1,210)	1:84:A:VAL:HG22	1:80:A:LEU:HA	11	0.14
(1,210)	1:84:A:VAL:HG23	1:80:A:LEU:HA	11	0.14
(1,204)	1:83:A:LYS:H	1:82:A:GLU:HA	1	0.14
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	2	0.14
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	3	0.14
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	4	0.14
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	3	0.14
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	3	0.14
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	8	0.14
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	8	0.14
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD1	13	0.14
(1,109)	1:53:A:ALA:H	1:56:A:PHE:HD2	13	0.14
(1,102)	1:49:A:LEU:H	1:49:A:LEU:HB2	10	0.14
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	3	0.14
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	4	0.14
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	4	0.14
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	8	0.14
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	14	0.14
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG21	2	0.14
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG22	2	0.14
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG23	2	0.14
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG21	2	0.14
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG22	2	0.14
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG23	2	0.14
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG21	2	0.14
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG22	2	0.14
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG23	2	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG21	2	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG22	2	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG23	2	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG21	2	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG22	2	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG23	2	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG21	2	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG22	2	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG23	2	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG21	2	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG22	2	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG23	2	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG21	2	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG22	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG23	2	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG21	2	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG22	2	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG23	2	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG21	12	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG22	12	0.14
(1,48)	1:20:A:VAL:HG11	1:24:A:ILE:HG23	12	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG21	12	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG22	12	0.14
(1,48)	1:20:A:VAL:HG12	1:24:A:ILE:HG23	12	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG21	12	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG22	12	0.14
(1,48)	1:20:A:VAL:HG13	1:24:A:ILE:HG23	12	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG21	12	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG22	12	0.14
(1,48)	1:20:A:VAL:HG21	1:24:A:ILE:HG23	12	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG21	12	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG22	12	0.14
(1,48)	1:20:A:VAL:HG22	1:24:A:ILE:HG23	12	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG21	12	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG22	12	0.14
(1,48)	1:20:A:VAL:HG23	1:24:A:ILE:HG23	12	0.14
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB1	8	0.14
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB2	8	0.14
(1,46)	1:20:A:VAL:H	1:16:A:ALA:HB3	8	0.14
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	3	0.14
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	3	0.14
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	3	0.14
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	8	0.14
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	8	0.14
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	8	0.14
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	8	0.14
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	8	0.14
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	8	0.14
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	8	0.14
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	8	0.14
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	8	0.14
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	3	0.13
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	3	0.13
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	3	0.13
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	3	0.13
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	3	0.13
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	7	0.13
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	7	0.13
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	7	0.13
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	7	0.13
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	7	0.13
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	7	0.13
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA2	5	0.13
(1,619)	1:180:A:LEU:HD21	1:94:A:GLY:HA3	5	0.13
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA2	5	0.13
(1,619)	1:180:A:LEU:HD22	1:94:A:GLY:HA3	5	0.13
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA2	5	0.13
(1,619)	1:180:A:LEU:HD23	1:94:A:GLY:HA3	5	0.13
(1,578)	1:111:A:LEU:HD11	1:179:A:TYR:HE1	12	0.13
(1,578)	1:111:A:LEU:HD11	1:179:A:TYR:HE2	12	0.13
(1,578)	1:111:A:LEU:HD12	1:179:A:TYR:HE1	12	0.13
(1,578)	1:111:A:LEU:HD12	1:179:A:TYR:HE2	12	0.13
(1,578)	1:111:A:LEU:HD13	1:179:A:TYR:HE1	12	0.13
(1,578)	1:111:A:LEU:HD13	1:179:A:TYR:HE2	12	0.13
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB2	11	0.13
(1,575)	1:102:A:LEU:H	1:97:A:TRP:HB3	11	0.13
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	1	0.13
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	1	0.13
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	1	0.13
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	1	0.13
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	1	0.13
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	1	0.13
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	12	0.13
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	12	0.13
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	12	0.13
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	12	0.13
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	12	0.13
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	12	0.13
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD1	6	0.13
(1,560)	1:63:A:VAL:HG11	1:105:A:PHE:HD2	6	0.13
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD1	6	0.13
(1,560)	1:63:A:VAL:HG12	1:105:A:PHE:HD2	6	0.13
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD1	6	0.13
(1,560)	1:63:A:VAL:HG13	1:105:A:PHE:HD2	6	0.13
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD2	11	0.13
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD3	11	0.13
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD2	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD3	11	0.13
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD2	11	0.13
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD3	11	0.13
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	12	0.13
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	12	0.13
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	12	0.13
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	12	0.13
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	12	0.13
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	12	0.13
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	12	0.13
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	12	0.13
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	12	0.13
(1,530)	1:16:A:ALA:HB1	1:24:A:ILE:HD11	11	0.13
(1,530)	1:16:A:ALA:HB1	1:24:A:ILE:HD12	11	0.13
(1,530)	1:16:A:ALA:HB1	1:24:A:ILE:HD13	11	0.13
(1,530)	1:16:A:ALA:HB2	1:24:A:ILE:HD11	11	0.13
(1,530)	1:16:A:ALA:HB2	1:24:A:ILE:HD12	11	0.13
(1,530)	1:16:A:ALA:HB2	1:24:A:ILE:HD13	11	0.13
(1,530)	1:16:A:ALA:HB3	1:24:A:ILE:HD11	11	0.13
(1,530)	1:16:A:ALA:HB3	1:24:A:ILE:HD12	11	0.13
(1,530)	1:16:A:ALA:HB3	1:24:A:ILE:HD13	11	0.13
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA2	8	0.13
(1,529)	1:14:A:SER:H	1:157:A:GLY:HA3	8	0.13
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	6	0.13
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	6	0.13
(1,517)	1:183:A:PHE:H	1:180:A:LEU:HA	2	0.13
(1,517)	1:183:A:PHE:H	1:180:A:LEU:HA	13	0.13
(1,517)	1:183:A:PHE:H	1:180:A:LEU:HA	15	0.13
(1,504)	1:178:A:LEU:HD11	1:175:A:ILE:HA	14	0.13
(1,504)	1:178:A:LEU:HD12	1:175:A:ILE:HA	14	0.13
(1,504)	1:178:A:LEU:HD13	1:175:A:ILE:HA	14	0.13
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	6	0.13
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	14	0.13
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	2	0.13
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	14	0.13
(1,453)	1:165:A:PHE:H	1:165:A:PHE:HB2	13	0.13
(1,450)	1:165:A:PHE:H	1:163:A:ALA:H	1	0.13
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	10	0.13
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	6	0.13
(1,418)	1:152:A:ALA:H	1:149:A:THR:HA	9	0.13
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	4	0.13
(1,393)	1:145:A:GLY:H	1:144:A:LEU:HA	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	14	0.13
(1,371)	1:140:A:LEU:H	1:137:A:LEU:H	9	0.13
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	3	0.13
(1,366)	1:139:A:MET:H	1:138:A:VAL:HB	11	0.13
(1,339)	1:128:A:SER:H	1:125:A:ILE:HA	9	0.13
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	3	0.13
(1,309)	1:118:A:ALA:HB1	1:115:A:TRP:HA	1	0.13
(1,309)	1:118:A:ALA:HB2	1:115:A:TRP:HA	1	0.13
(1,309)	1:118:A:ALA:HB3	1:115:A:TRP:HA	1	0.13
(1,306)	1:118:A:ALA:H	1:115:A:TRP:HA	9	0.13
(1,303)	1:115:A:TRP:H	1:114:A:LEU:H	2	0.13
(1,302)	1:114:A:LEU:H	1:115:A:TRP:H	2	0.13
(1,299)	1:114:A:LEU:H	1:114:A:LEU:HB3	2	0.13
(1,264)	1:108:A:GLY:H	1:107:A:PHE:H	11	0.13
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	14	0.13
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	14	0.13
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	14	0.13
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	7	0.13
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	12	0.13
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	12	0.13
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	12	0.13
(1,86)	1:42:A:LEU:H	1:41:A:GLY:HA2	3	0.13
(1,86)	1:42:A:LEU:H	1:41:A:GLY:HA2	15	0.13
(1,85)	1:42:A:LEU:H	1:39:A:VAL:HA	10	0.13
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	7	0.13
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	11	0.13
(1,52)	1:26:A:ALA:HB1	1:24:A:ILE:H	8	0.13
(1,52)	1:26:A:ALA:HB2	1:24:A:ILE:H	8	0.13
(1,52)	1:26:A:ALA:HB3	1:24:A:ILE:H	8	0.13
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	12	0.13
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	12	0.13
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	12	0.13
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB1	14	0.13
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB2	14	0.13
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB3	14	0.13
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	4	0.13
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	4	0.13
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	4	0.13
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	4	0.13
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	4	0.13
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	4	0.13
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	4	0.13
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	4	0.13
(1,621)	1:188:A:VAL:HG11	1:49:A:LEU:H	11	0.12
(1,621)	1:188:A:VAL:HG12	1:49:A:LEU:H	11	0.12
(1,621)	1:188:A:VAL:HG13	1:49:A:LEU:H	11	0.12
(1,621)	1:188:A:VAL:HG21	1:49:A:LEU:H	11	0.12
(1,621)	1:188:A:VAL:HG22	1:49:A:LEU:H	11	0.12
(1,621)	1:188:A:VAL:HG23	1:49:A:LEU:H	11	0.12
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA2	3	0.12
(1,610)	1:173:A:GLY:H	1:145:A:GLY:HA3	3	0.12
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD11	4	0.12
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD12	4	0.12
(1,608)	1:164:A:ASN:H	1:24:A:ILE:HD13	4	0.12
(1,607)	1:161:A:VAL:HG11	1:152:A:ALA:HA	13	0.12
(1,607)	1:161:A:VAL:HG12	1:152:A:ALA:HA	13	0.12
(1,607)	1:161:A:VAL:HG13	1:152:A:ALA:HA	13	0.12
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD11	9	0.12
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD12	9	0.12
(1,605)	1:161:A:VAL:H	1:24:A:ILE:HD13	9	0.12
(1,603)	1:150:A:ILE:HD11	1:123:A:ALA:HB1	8	0.12
(1,603)	1:150:A:ILE:HD11	1:123:A:ALA:HB2	8	0.12
(1,603)	1:150:A:ILE:HD11	1:123:A:ALA:HB3	8	0.12
(1,603)	1:150:A:ILE:HD12	1:123:A:ALA:HB1	8	0.12
(1,603)	1:150:A:ILE:HD12	1:123:A:ALA:HB2	8	0.12
(1,603)	1:150:A:ILE:HD12	1:123:A:ALA:HB3	8	0.12
(1,603)	1:150:A:ILE:HD13	1:123:A:ALA:HB1	8	0.12
(1,603)	1:150:A:ILE:HD13	1:123:A:ALA:HB2	8	0.12
(1,603)	1:150:A:ILE:HD13	1:123:A:ALA:HB3	8	0.12
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD1	8	0.12
(1,594)	1:125:A:ILE:HD11	1:142:A:TYR:HD2	8	0.12
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD1	8	0.12
(1,594)	1:125:A:ILE:HD12	1:142:A:TYR:HD2	8	0.12
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD1	8	0.12
(1,594)	1:125:A:ILE:HD13	1:142:A:TYR:HD2	8	0.12
(1,593)	1:123:A:ALA:HB1	1:150:A:ILE:HD11	8	0.12
(1,593)	1:123:A:ALA:HB1	1:150:A:ILE:HD12	8	0.12
(1,593)	1:123:A:ALA:HB1	1:150:A:ILE:HD13	8	0.12
(1,593)	1:123:A:ALA:HB2	1:150:A:ILE:HD11	8	0.12
(1,593)	1:123:A:ALA:HB2	1:150:A:ILE:HD12	8	0.12
(1,593)	1:123:A:ALA:HB2	1:150:A:ILE:HD13	8	0.12
(1,593)	1:123:A:ALA:HB3	1:150:A:ILE:HD11	8	0.12
(1,593)	1:123:A:ALA:HB3	1:150:A:ILE:HD12	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:123:A:ALA:HB3	1:150:A:ILE:HD13	8	0.12
(1,592)	1:119:A:ILE:HD11	1:174:A:ALA:HA	15	0.12
(1,592)	1:119:A:ILE:HD12	1:174:A:ALA:HA	15	0.12
(1,592)	1:119:A:ILE:HD13	1:174:A:ALA:HA	15	0.12
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB1	3	0.12
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB2	3	0.12
(1,590)	1:119:A:ILE:H	1:174:A:ALA:HB3	3	0.12
(1,587)	1:118:A:ALA:HB1	1:39:A:VAL:HB	10	0.12
(1,587)	1:118:A:ALA:HB2	1:39:A:VAL:HB	10	0.12
(1,587)	1:118:A:ALA:HB3	1:39:A:VAL:HB	10	0.12
(1,585)	1:118:A:ALA:H	1:39:A:VAL:HA	15	0.12
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	7	0.12
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	7	0.12
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	7	0.12
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	7	0.12
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	7	0.12
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	7	0.12
(1,559)	1:50:A:GLY:H	1:182:A:TYR:HE1	4	0.12
(1,559)	1:50:A:GLY:H	1:182:A:TYR:HE2	4	0.12
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	7	0.12
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	7	0.12
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	7	0.12
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	7	0.12
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	7	0.12
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	7	0.12
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	3	0.12
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	3	0.12
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	3	0.12
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	3	0.12
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	3	0.12
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	3	0.12
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	11	0.12
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	11	0.12
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	11	0.12
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	11	0.12
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	11	0.12
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	11	0.12
(1,536)	1:27:A:GLY:H	1:12:A:VAL:HG11	6	0.12
(1,536)	1:27:A:GLY:H	1:12:A:VAL:HG12	6	0.12
(1,536)	1:27:A:GLY:H	1:12:A:VAL:HG13	6	0.12
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE2	6	0.12
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE2	6	0.12
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE3	6	0.12
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE2	6	0.12
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE3	6	0.12
(1,531)	1:16:A:ALA:HB1	1:27:A:GLY:H	12	0.12
(1,531)	1:16:A:ALA:HB2	1:27:A:GLY:H	12	0.12
(1,531)	1:16:A:ALA:HB3	1:27:A:GLY:H	12	0.12
(1,517)	1:183:A:PHE:H	1:180:A:LEU:HA	5	0.12
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	4	0.12
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	8	0.12
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	10	0.12
(1,490)	1:174:A:ALA:H	1:171:A:VAL:HA	7	0.12
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	4	0.12
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	7	0.12
(1,480)	1:172:A:THR:H	1:169:A:ARG:HA	11	0.12
(1,476)	1:171:A:VAL:H	1:168:A:ILE:HA	5	0.12
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	3	0.12
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	6	0.12
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	15	0.12
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	2	0.12
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	2	0.12
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD1	7	0.12
(1,463)	1:168:A:ILE:H	1:165:A:PHE:HD2	7	0.12
(1,448)	1:164:A:ASN:H	1:163:A:ALA:H	11	0.12
(1,447)	1:163:A:ALA:H	1:164:A:ASN:H	11	0.12
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	5	0.12
(1,429)	1:154:A:PHE:H	1:151:A:ALA:HA	6	0.12
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	1	0.12
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	1	0.12
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	1	0.12
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	1	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	1	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	1	0.12
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	6	0.12
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	6	0.12
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	6	0.12
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	6	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	6	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	6	0.12
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	13	0.12
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	13	0.12
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	13	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	13	0.12
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	13	0.12
(1,423)	1:153:A:VAL:H	1:150:A:ILE:HA	11	0.12
(1,423)	1:153:A:VAL:H	1:150:A:ILE:HA	14	0.12
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	6	0.12
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	9	0.12
(1,413)	1:151:A:ALA:H	1:148:A:VAL:HA	12	0.12
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB2	13	0.12
(1,412)	1:150:A:ILE:HG21	1:154:A:PHE:HB3	13	0.12
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB2	13	0.12
(1,412)	1:150:A:ILE:HG22	1:154:A:PHE:HB3	13	0.12
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB2	13	0.12
(1,412)	1:150:A:ILE:HG23	1:154:A:PHE:HB3	13	0.12
(1,402)	1:148:A:VAL:H	1:147:A:ALA:HA	2	0.12
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	13	0.12
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	15	0.12
(1,393)	1:145:A:GLY:H	1:144:A:LEU:HA	6	0.12
(1,393)	1:145:A:GLY:H	1:144:A:LEU:HA	8	0.12
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	4	0.12
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD1	3	0.12
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD2	3	0.12
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD1	3	0.12
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD2	3	0.12
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD1	3	0.12
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD2	3	0.12
(1,339)	1:128:A:SER:H	1:125:A:ILE:HA	8	0.12
(1,335)	1:127:A:ILE:H	1:126:A:ALA:HA	6	0.12
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	12	0.12
(1,328)	1:126:A:ALA:H	1:123:A:ALA:HA	14	0.12
(1,310)	1:119:A:ILE:HG21	1:123:A:ALA:H	2	0.12
(1,310)	1:119:A:ILE:HG22	1:123:A:ALA:H	2	0.12
(1,310)	1:119:A:ILE:HG23	1:123:A:ALA:H	2	0.12
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	1	0.12
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	15	0.12
(1,243)	1:91:A:MET:H	1:88:A:ALA:HA	14	0.12
(1,208)	1:84:A:VAL:HG11	1:81:A:ASP:HA	7	0.12
(1,208)	1:84:A:VAL:HG12	1:81:A:ASP:HA	7	0.12
(1,208)	1:84:A:VAL:HG13	1:81:A:ASP:HA	7	0.12
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	3	0.12
(1,203)	1:82:A:GLU:H	1:85:A:SER:H	13	0.12
(1,166)	1:72:A:ALA:H	1:74:A:ILE:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	12	0.12
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	14	0.12
(1,121)	1:58:A:GLY:H	1:56:A:PHE:H	15	0.12
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	3	0.12
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	3	0.12
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	3	0.12
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	10	0.12
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	10	0.12
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	10	0.12
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB1	5	0.12
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB2	5	0.12
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB3	5	0.12
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB1	14	0.12
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB2	14	0.12
(1,110)	1:56:A:PHE:H	1:53:A:ALA:HB3	14	0.12
(1,101)	1:49:A:LEU:H	1:49:A:LEU:HB3	5	0.12
(1,85)	1:42:A:LEU:H	1:39:A:VAL:HA	9	0.12
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	10	0.12
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	2	0.12
(1,32)	1:12:A:VAL:H	1:9:A:ILE:HA	6	0.12
(1,620)	1:181:A:ALA:HB1	1:138:A:VAL:HA	1	0.11
(1,620)	1:181:A:ALA:HB2	1:138:A:VAL:HA	1	0.11
(1,620)	1:181:A:ALA:HB3	1:138:A:VAL:HA	1	0.11
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG2	8	0.11
(1,616)	1:176:A:VAL:H	1:90:A:ARG:HG3	8	0.11
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA2	15	0.11
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA3	15	0.11
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD11	2	0.11
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD12	2	0.11
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD13	2	0.11
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD11	2	0.11
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD12	2	0.11
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD13	2	0.11
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD11	2	0.11
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD12	2	0.11
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD13	2	0.11
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD11	14	0.11
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD12	14	0.11
(1,606)	1:161:A:VAL:HG11	1:24:A:ILE:HD13	14	0.11
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD11	14	0.11
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD12	14	0.11
(1,606)	1:161:A:VAL:HG12	1:24:A:ILE:HD13	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD11	14	0.11
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD12	14	0.11
(1,606)	1:161:A:VAL:HG13	1:24:A:ILE:HD13	14	0.11
(1,589)	1:118:A:ALA:HB1	1:175:A:ILE:HA	10	0.11
(1,589)	1:118:A:ALA:HB2	1:175:A:ILE:HA	10	0.11
(1,589)	1:118:A:ALA:HB3	1:175:A:ILE:HA	10	0.11
(1,581)	1:112:A:ALA:HB1	1:95:A:LEU:HA	14	0.11
(1,581)	1:112:A:ALA:HB2	1:95:A:LEU:HA	14	0.11
(1,581)	1:112:A:ALA:HB3	1:95:A:LEU:HA	14	0.11
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	5	0.11
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	5	0.11
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	5	0.11
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	5	0.11
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	5	0.11
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	5	0.11
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE1	12	0.11
(1,577)	1:110:A:LEU:HD21	1:105:A:PHE:HE2	12	0.11
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE1	12	0.11
(1,577)	1:110:A:LEU:HD22	1:105:A:PHE:HE2	12	0.11
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE1	12	0.11
(1,577)	1:110:A:LEU:HD23	1:105:A:PHE:HE2	12	0.11
(1,573)	1:88:A:ALA:HB1	1:76:A:LEU:HG	7	0.11
(1,573)	1:88:A:ALA:HB2	1:76:A:LEU:HG	7	0.11
(1,573)	1:88:A:ALA:HB3	1:76:A:LEU:HG	7	0.11
(1,573)	1:88:A:ALA:HB1	1:76:A:LEU:HG	15	0.11
(1,573)	1:88:A:ALA:HB2	1:76:A:LEU:HG	15	0.11
(1,573)	1:88:A:ALA:HB3	1:76:A:LEU:HG	15	0.11
(1,569)	1:76:A:LEU:HD11	1:87:A:PHE:HD1	6	0.11
(1,569)	1:76:A:LEU:HD11	1:87:A:PHE:HD2	6	0.11
(1,569)	1:76:A:LEU:HD12	1:87:A:PHE:HD1	6	0.11
(1,569)	1:76:A:LEU:HD12	1:87:A:PHE:HD2	6	0.11
(1,569)	1:76:A:LEU:HD13	1:87:A:PHE:HD1	6	0.11
(1,569)	1:76:A:LEU:HD13	1:87:A:PHE:HD2	6	0.11
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD11	8	0.11
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD12	8	0.11
(1,565)	1:68:A:LEU:HD21	1:38:A:ILE:HD13	8	0.11
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD11	8	0.11
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD12	8	0.11
(1,565)	1:68:A:LEU:HD22	1:38:A:ILE:HD13	8	0.11
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD11	8	0.11
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD12	8	0.11
(1,565)	1:68:A:LEU:HD23	1:38:A:ILE:HD13	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD1	14	0.11
(1,561)	1:63:A:VAL:HG21	1:105:A:PHE:HD2	14	0.11
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD1	14	0.11
(1,561)	1:63:A:VAL:HG22	1:105:A:PHE:HD2	14	0.11
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD1	14	0.11
(1,561)	1:63:A:VAL:HG23	1:105:A:PHE:HD2	14	0.11
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG2	4	0.11
(1,555)	1:48:A:ILE:HG21	1:61:A:ARG:HG3	4	0.11
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG2	4	0.11
(1,555)	1:48:A:ILE:HG22	1:61:A:ARG:HG3	4	0.11
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG2	4	0.11
(1,555)	1:48:A:ILE:HG23	1:61:A:ARG:HG3	4	0.11
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD11	2	0.11
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD12	2	0.11
(1,547)	1:42:A:LEU:HD11	1:178:A:LEU:HD13	2	0.11
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD11	2	0.11
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD12	2	0.11
(1,547)	1:42:A:LEU:HD12	1:178:A:LEU:HD13	2	0.11
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD11	2	0.11
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD12	2	0.11
(1,547)	1:42:A:LEU:HD13	1:178:A:LEU:HD13	2	0.11
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD2	4	0.11
(1,544)	1:40:A:ALA:HB1	1:121:A:PRO:HD3	4	0.11
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD2	4	0.11
(1,544)	1:40:A:ALA:HB2	1:121:A:PRO:HD3	4	0.11
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD2	4	0.11
(1,544)	1:40:A:ALA:HB3	1:121:A:PRO:HD3	4	0.11
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD1	10	0.11
(1,540)	1:38:A:ILE:HG21	1:71:A:PHE:HD2	10	0.11
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD1	10	0.11
(1,540)	1:38:A:ILE:HG22	1:71:A:PHE:HD2	10	0.11
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD1	10	0.11
(1,540)	1:38:A:ILE:HG23	1:71:A:PHE:HD2	10	0.11
(1,537)	1:27:A:GLY:H	1:12:A:VAL:HG21	14	0.11
(1,537)	1:27:A:GLY:H	1:12:A:VAL:HG22	14	0.11
(1,537)	1:27:A:GLY:H	1:12:A:VAL:HG23	14	0.11
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG21	8	0.11
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG22	8	0.11
(1,535)	1:26:A:ALA:HB1	1:153:A:VAL:HG23	8	0.11
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG21	8	0.11
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG22	8	0.11
(1,535)	1:26:A:ALA:HB2	1:153:A:VAL:HG23	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG21	8	0.11
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG22	8	0.11
(1,535)	1:26:A:ALA:HB3	1:153:A:VAL:HG23	8	0.11
(1,531)	1:16:A:ALA:HB1	1:27:A:GLY:H	9	0.11
(1,531)	1:16:A:ALA:HB2	1:27:A:GLY:H	9	0.11
(1,531)	1:16:A:ALA:HB3	1:27:A:GLY:H	9	0.11
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	3	0.11
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	3	0.11
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE1	10	0.11
(1,526)	1:10:A:LEU:H	1:36:A:PHE:HE2	10	0.11
(1,517)	1:183:A:PHE:H	1:180:A:LEU:HA	3	0.11
(1,517)	1:183:A:PHE:H	1:180:A:LEU:HA	8	0.11
(1,512)	1:182:A:TYR:H	1:179:A:TYR:HA	1	0.11
(1,506)	1:180:A:LEU:H	1:177:A:LEU:HA	14	0.11
(1,504)	1:178:A:LEU:HD11	1:175:A:ILE:HA	3	0.11
(1,504)	1:178:A:LEU:HD12	1:175:A:ILE:HA	3	0.11
(1,504)	1:178:A:LEU:HD13	1:175:A:ILE:HA	3	0.11
(1,490)	1:174:A:ALA:H	1:171:A:VAL:HA	6	0.11
(1,486)	1:173:A:GLY:H	1:170:A:LYS:HA	12	0.11
(1,476)	1:171:A:VAL:H	1:168:A:ILE:HA	12	0.11
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	9	0.11
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD21	5	0.11
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD22	5	0.11
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD21	5	0.11
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD22	5	0.11
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD21	5	0.11
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD22	5	0.11
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD21	5	0.11
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD22	5	0.11
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD21	5	0.11
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD22	5	0.11
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD21	5	0.11
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD22	5	0.11
(1,453)	1:165:A:PHE:H	1:165:A:PHE:HB2	11	0.11
(1,448)	1:164:A:ASN:H	1:163:A:ALA:H	8	0.11
(1,447)	1:163:A:ALA:H	1:164:A:ASN:H	8	0.11
(1,446)	1:163:A:ALA:H	1:162:A:LYS:H	10	0.11
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	15	0.11
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	15	0.11
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	7	0.11
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	7	0.11
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	7	0.11
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	7	0.11
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	7	0.11
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	11	0.11
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	11	0.11
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	11	0.11
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	11	0.11
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	11	0.11
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	11	0.11
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	12	0.11
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	12	0.11
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	12	0.11
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	12	0.11
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	12	0.11
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	12	0.11
(1,423)	1:153:A:VAL:H	1:150:A:ILE:HA	1	0.11
(1,423)	1:153:A:VAL:H	1:150:A:ILE:HA	12	0.11
(1,400)	1:147:A:ALA:H	1:149:A:THR:H	8	0.11
(1,396)	1:147:A:ALA:H	1:146:A:MET:HA	13	0.11
(1,371)	1:140:A:LEU:H	1:137:A:LEU:H	7	0.11
(1,339)	1:128:A:SER:H	1:125:A:ILE:HA	5	0.11
(1,335)	1:127:A:ILE:H	1:126:A:ALA:HA	3	0.11
(1,335)	1:127:A:ILE:H	1:126:A:ALA:HA	4	0.11
(1,335)	1:127:A:ILE:H	1:126:A:ALA:HA	8	0.11
(1,335)	1:127:A:ILE:H	1:126:A:ALA:HA	10	0.11
(1,335)	1:127:A:ILE:H	1:126:A:ALA:HA	11	0.11
(1,319)	1:124:A:GLY:H	1:123:A:ALA:HA	13	0.11
(1,305)	1:115:A:TRP:H	1:116:A:LEU:H	7	0.11
(1,305)	1:115:A:TRP:H	1:116:A:LEU:H	10	0.11
(1,290)	1:113:A:PHE:H	1:110:A:LEU:HA	7	0.11
(1,289)	1:112:A:ALA:H	1:114:A:LEU:H	9	0.11
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG12	1	0.11
(1,234)	1:89:A:SER:H	1:86:A:ILE:HG13	1	0.11
(1,202)	1:82:A:GLU:H	1:84:A:VAL:H	13	0.11
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	8	0.11
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	8	0.11
(1,133)	1:62:A:VAL:H	1:59:A:PHE:HA	9	0.11
(1,116)	1:57:A:PHE:H	1:56:A:PHE:H	13	0.11
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	8	0.11
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	8	0.11
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	8	0.11
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB1	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB2	14	0.11
(1,114)	1:57:A:PHE:H	1:53:A:ALA:HB3	14	0.11
(1,107)	1:50:A:GLY:H	1:51:A:TYR:H	1	0.11
(1,98)	1:49:A:LEU:H	1:48:A:ILE:HA	6	0.11
(1,86)	1:42:A:LEU:H	1:41:A:GLY:HA2	10	0.11
(1,73)	1:39:A:VAL:H	1:36:A:PHE:HA	6	0.11
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	1	0.11
(1,71)	1:38:A:ILE:H	1:40:A:ALA:H	13	0.11
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	5	0.11
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	5	0.11
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	5	0.11
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	9	0.11
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	9	0.11
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	9	0.11
(1,20)	1:9:A:ILE:H	1:6:A:ALA:HA	8	0.11
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB1	9	0.11
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB2	9	0.11
(1,13)	1:8:A:GLY:H	1:4:A:ALA:HB3	9	0.11
(1,1)	1:4:A:ALA:H	1:1:A:GLN:HG2	14	0.11
(1,1)	1:4:A:ALA:H	1:1:A:GLN:HG3	14	0.11
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA2	2	0.1
(1,614)	1:174:A:ALA:H	1:145:A:GLY:HA3	2	0.1
(1,607)	1:161:A:VAL:HG11	1:152:A:ALA:HA	5	0.1
(1,607)	1:161:A:VAL:HG12	1:152:A:ALA:HA	5	0.1
(1,607)	1:161:A:VAL:HG13	1:152:A:ALA:HA	5	0.1
(1,595)	1:126:A:ALA:HB1	1:142:A:TYR:HD1	14	0.1
(1,595)	1:126:A:ALA:HB1	1:142:A:TYR:HD2	14	0.1
(1,595)	1:126:A:ALA:HB2	1:142:A:TYR:HD1	14	0.1
(1,595)	1:126:A:ALA:HB2	1:142:A:TYR:HD2	14	0.1
(1,595)	1:126:A:ALA:HB3	1:142:A:TYR:HD1	14	0.1
(1,595)	1:126:A:ALA:HB3	1:142:A:TYR:HD2	14	0.1
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD1	7	0.1
(1,538)	1:27:A:GLY:H	1:160:A:PHE:HD2	7	0.1
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE2	8	0.1
(1,533)	1:24:A:ILE:HG21	1:170:A:LYS:HE3	8	0.1
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE2	8	0.1
(1,533)	1:24:A:ILE:HG22	1:170:A:LYS:HE3	8	0.1
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE2	8	0.1
(1,533)	1:24:A:ILE:HG23	1:170:A:LYS:HE3	8	0.1
(1,531)	1:16:A:ALA:HB1	1:27:A:GLY:H	10	0.1
(1,531)	1:16:A:ALA:HB2	1:27:A:GLY:H	10	0.1
(1,531)	1:16:A:ALA:HB3	1:27:A:GLY:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:178:A:LEU:HD11	1:175:A:ILE:HA	11	0.1
(1,504)	1:178:A:LEU:HD12	1:175:A:ILE:HA	11	0.1
(1,504)	1:178:A:LEU:HD13	1:175:A:ILE:HA	11	0.1
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD11	1	0.1
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD12	1	0.1
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD13	1	0.1
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD21	1	0.1
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD22	1	0.1
(1,496)	1:175:A:ILE:HD11	1:178:A:LEU:HD23	1	0.1
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD11	1	0.1
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD12	1	0.1
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD13	1	0.1
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD21	1	0.1
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD22	1	0.1
(1,496)	1:175:A:ILE:HD12	1:178:A:LEU:HD23	1	0.1
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD11	1	0.1
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD12	1	0.1
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD13	1	0.1
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD21	1	0.1
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD22	1	0.1
(1,496)	1:175:A:ILE:HD13	1:178:A:LEU:HD23	1	0.1
(1,481)	1:172:A:THR:H	1:171:A:VAL:HA	2	0.1
(1,471)	1:169:A:ARG:H	1:171:A:VAL:H	12	0.1
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD21	13	0.1
(1,461)	1:167:A:LEU:HD11	1:164:A:ASN:HD22	13	0.1
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD21	13	0.1
(1,461)	1:167:A:LEU:HD12	1:164:A:ASN:HD22	13	0.1
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD21	13	0.1
(1,461)	1:167:A:LEU:HD13	1:164:A:ASN:HD22	13	0.1
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD21	13	0.1
(1,461)	1:167:A:LEU:HD21	1:164:A:ASN:HD22	13	0.1
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD21	13	0.1
(1,461)	1:167:A:LEU:HD22	1:164:A:ASN:HD22	13	0.1
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD21	13	0.1
(1,461)	1:167:A:LEU:HD23	1:164:A:ASN:HD22	13	0.1
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE1	10	0.1
(1,440)	1:156:A:MET:H	1:160:A:PHE:HE2	10	0.1
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD1	9	0.1
(1,428)	1:153:A:VAL:HG21	1:154:A:PHE:HD2	9	0.1
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD1	9	0.1
(1,428)	1:153:A:VAL:HG22	1:154:A:PHE:HD2	9	0.1
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD1	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:153:A:VAL:HG23	1:154:A:PHE:HD2	9	0.1
(1,402)	1:148:A:VAL:H	1:147:A:ALA:HA	4	0.1
(1,402)	1:148:A:VAL:H	1:147:A:ALA:HA	7	0.1
(1,401)	1:148:A:VAL:H	1:146:A:MET:H	14	0.1
(1,392)	1:145:A:GLY:H	1:142:A:TYR:HA	9	0.1
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD1	12	0.1
(1,364)	1:138:A:VAL:HG21	1:142:A:TYR:HD2	12	0.1
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD1	12	0.1
(1,364)	1:138:A:VAL:HG22	1:142:A:TYR:HD2	12	0.1
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD1	12	0.1
(1,364)	1:138:A:VAL:HG23	1:142:A:TYR:HD2	12	0.1
(1,339)	1:128:A:SER:H	1:125:A:ILE:HA	13	0.1
(1,297)	1:114:A:LEU:H	1:113:A:PHE:HA	10	0.1
(1,225)	1:87:A:PHE:H	1:87:A:PHE:HB2	8	0.1
(1,210)	1:84:A:VAL:HG21	1:80:A:LEU:HA	10	0.1
(1,210)	1:84:A:VAL:HG22	1:80:A:LEU:HA	10	0.1
(1,210)	1:84:A:VAL:HG23	1:80:A:LEU:HA	10	0.1
(1,178)	1:75:A:LEU:H	1:72:A:ALA:HA	7	0.1
(1,138)	1:63:A:VAL:H	1:60:A:PHE:HA	3	0.1
(1,137)	1:63:A:VAL:H	1:59:A:PHE:HD1	1	0.1
(1,137)	1:63:A:VAL:H	1:59:A:PHE:HD2	1	0.1
(1,86)	1:42:A:LEU:H	1:41:A:GLY:HA2	5	0.1
(1,86)	1:42:A:LEU:H	1:41:A:GLY:HA2	9	0.1
(1,85)	1:42:A:LEU:H	1:39:A:VAL:HA	11	0.1
(1,77)	1:40:A:ALA:H	1:37:A:LEU:HA	12	0.1
(1,73)	1:39:A:VAL:H	1:36:A:PHE:HA	3	0.1
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG21	11	0.1
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG22	11	0.1
(1,53)	1:26:A:ALA:HB1	1:24:A:ILE:HG23	11	0.1
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG21	11	0.1
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG22	11	0.1
(1,53)	1:26:A:ALA:HB2	1:24:A:ILE:HG23	11	0.1
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG21	11	0.1
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG22	11	0.1
(1,53)	1:26:A:ALA:HB3	1:24:A:ILE:HG23	11	0.1
(1,50)	1:24:A:ILE:HD11	1:20:A:VAL:H	7	0.1
(1,50)	1:24:A:ILE:HD12	1:20:A:VAL:H	7	0.1
(1,50)	1:24:A:ILE:HD13	1:20:A:VAL:H	7	0.1
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	1	0.1
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	1	0.1
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	1	0.1
(1,45)	1:17:A:VAL:HG11	1:21:A:VAL:H	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:17:A:VAL:HG12	1:21:A:VAL:H	6	0.1
(1,45)	1:17:A:VAL:HG13	1:21:A:VAL:H	6	0.1
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD21	13	0.1
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD22	13	0.1
(1,3)	1:4:A:ALA:HB1	1:7:A:LEU:HD23	13	0.1
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD21	13	0.1
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD22	13	0.1
(1,3)	1:4:A:ALA:HB2	1:7:A:LEU:HD23	13	0.1
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD21	13	0.1
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD22	13	0.1
(1,3)	1:4:A:ALA:HB3	1:7:A:LEU:HD23	13	0.1

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

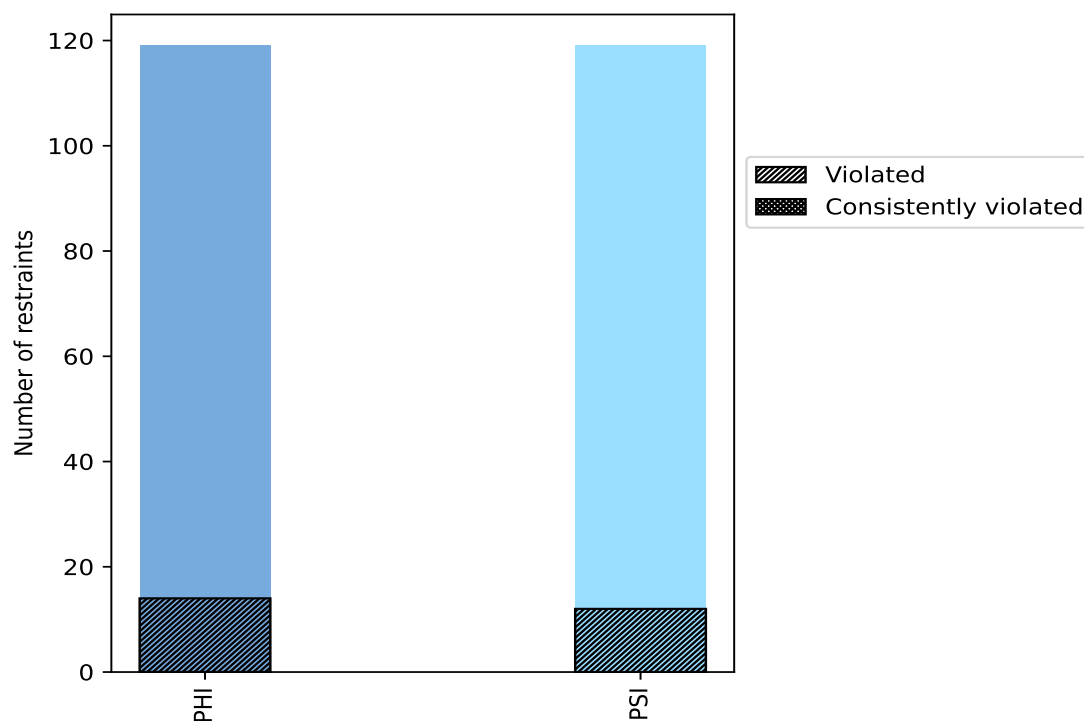
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	119	50.0	14	11.8	5.9	0	0.0	0.0
PSI	119	50.0	12	10.1	5.0	0	0.0	0.0
Total	238	100.0	26	10.9	10.9	0	0.0	0.0

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

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



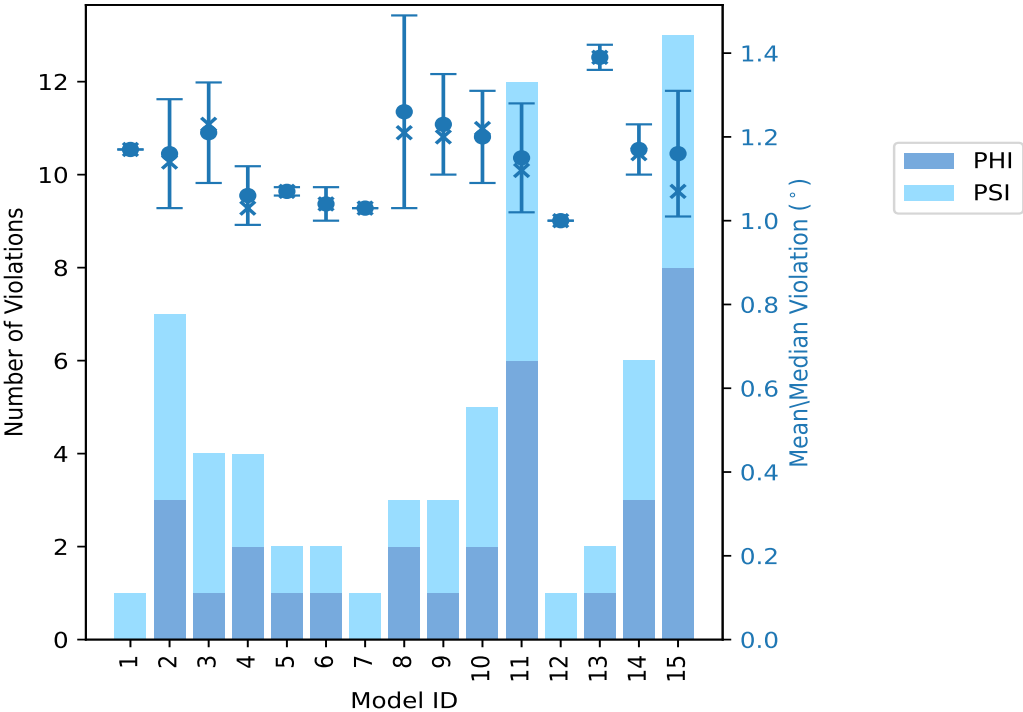
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	1.17	1.17	0.0	1.17
2	3	4	7	1.16	1.38	0.13	1.14
3	1	3	4	1.21	1.33	0.12	1.23
4	2	2	4	1.06	1.19	0.07	1.03
5	1	1	2	1.07	1.08	0.01	1.07
6	1	1	2	1.04	1.08	0.04	1.04
7	0	1	1	1.03	1.03	0.0	1.03
8	2	1	3	1.26	1.57	0.23	1.21
9	1	2	3	1.23	1.38	0.12	1.2
10	2	3	5	1.2	1.34	0.11	1.22
11	6	6	12	1.15	1.36	0.13	1.12
12	0	1	1	1.0	1.0	0.0	1.0
13	1	1	2	1.39	1.42	0.03	1.39
14	3	3	6	1.17	1.28	0.06	1.16
15	8	5	13	1.16	1.49	0.15	1.07

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

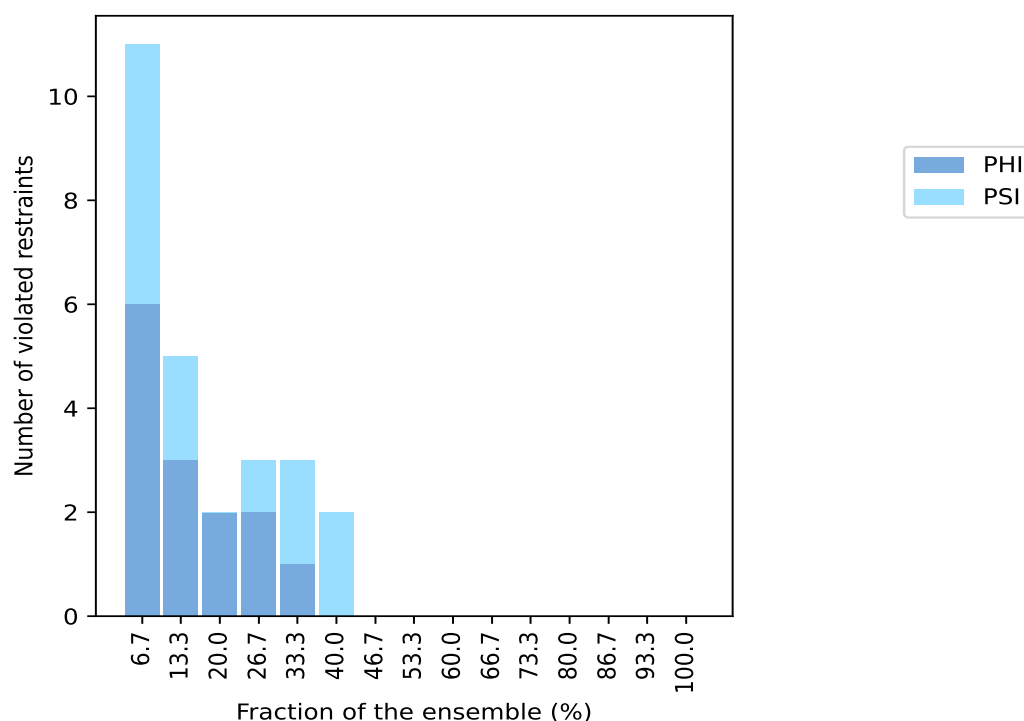
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	5	11	1	6.7
3	2	5	2	13.3
2	0	2	3	20.0
2	1	3	4	26.7
1	2	3	5	33.3
0	2	2	6	40.0
0	0	0	7	46.7
0	0	0	8	53.3
0	0	0	9	60.0
0	0	0	10	66.7
0	0	0	11	73.3
0	0	0	12	80.0
0	0	0	13	86.7
0	0	0	14	93.3
0	0	0	15	100.0

¹ Number of models with violations

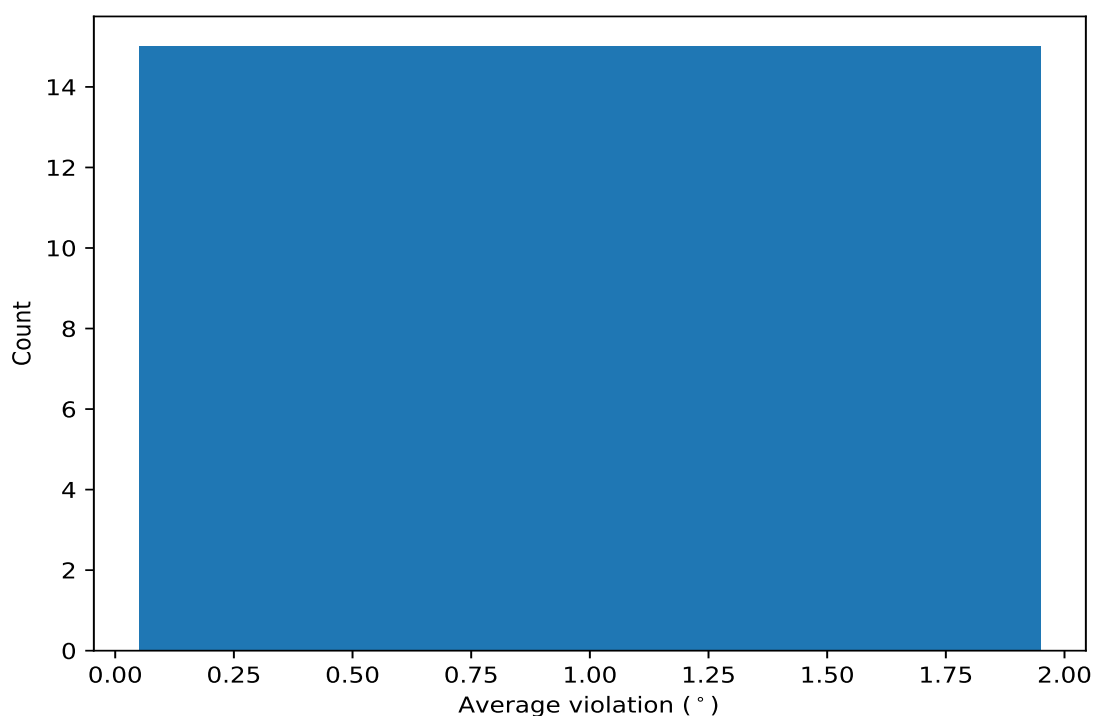
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

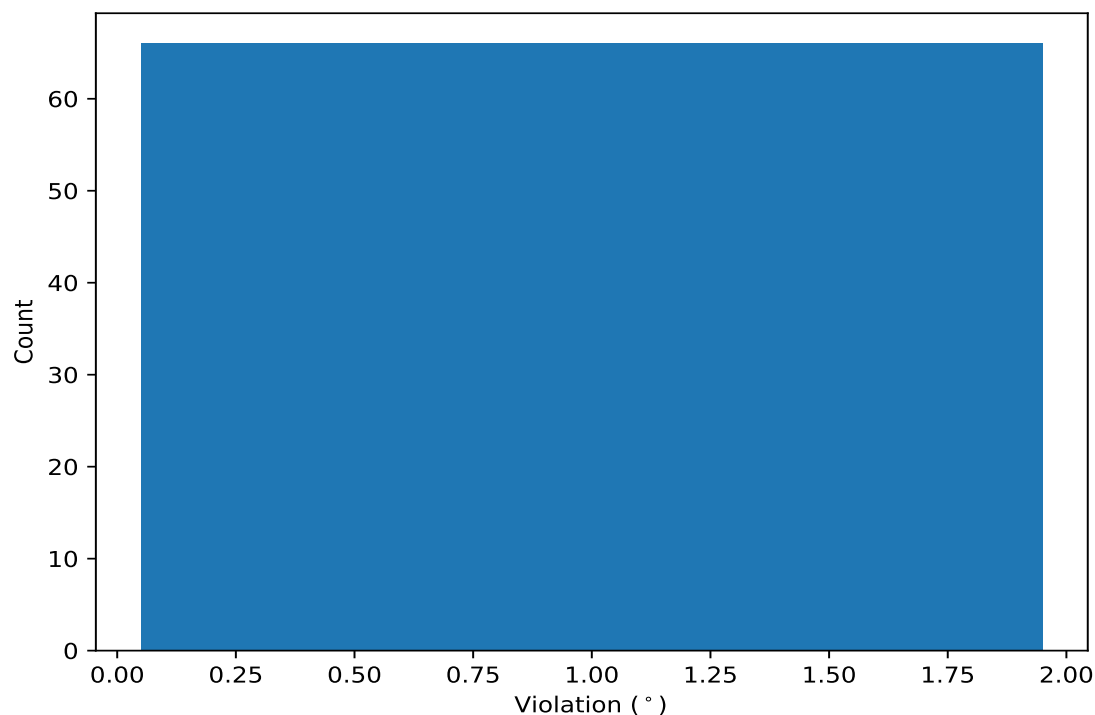
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(2,12)	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	1:114:A:LEU:N	6	1.28	0.19	1.27
(1,180)	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	1:176:A:VAL:N	6	1.22	0.15	1.27
(1,46)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:SER:N	5	1.29	0.15	1.33
(1,66)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:VAL:N	5	1.18	0.09	1.19
(1,67)	1:62:A:VAL:C	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	5	1.14	0.13	1.08
(1,47)	1:44:A:ILE:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	4	1.22	0.07	1.21
(2,22)	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1:121:A:PRO:N	4	1.14	0.08	1.16
(1,179)	1:174:A:ALA:C	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	4	1.06	0.05	1.04
(2,13)	1:113:A:PHE:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	3	1.3	0.07	1.34
(1,175)	1:172:A:THR:C	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	3	1.01	0.0	1.01
(1,45)	1:43:A:THR:C	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	2	1.23	0.1	1.23
(1,65)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	2	1.2	0.1	1.2
(1,181)	1:175:A:ILE:C	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	2	1.18	0.02	1.18
(1,182)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:LEU:N	2	1.14	0.08	1.14
(1,134)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:GLY:N	2	1.04	0.04	1.04

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,12)	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	1:114:A:LEU:N	8	1.57
(1,46)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:SER:N	15	1.49
(2,12)	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	1:114:A:LEU:N	13	1.42
(1,180)	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	1:176:A:VAL:N	9	1.38
(1,67)	1:62:A:VAL:C	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	2	1.38
(2,13)	1:113:A:PHE:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	13	1.36
(2,12)	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	1:114:A:LEU:N	11	1.36
(2,13)	1:113:A:PHE:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	11	1.34
(1,180)	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	1:176:A:VAL:N	11	1.34
(1,46)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:SER:N	10	1.34
(1,180)	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	1:176:A:VAL:N	3	1.33
(1,46)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:SER:N	3	1.33
(1,45)	1:43:A:THR:C	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	15	1.33
(1,65)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	15	1.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,66)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:VAL:N	2	1.3
(1,47)	1:44:A:ILE:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	15	1.3
(1,46)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:SER:N	14	1.28
(1,47)	1:44:A:ILE:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	10	1.27
(1,66)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:VAL:N	15	1.24
(2,22)	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1:121:A:PRO:N	10	1.22
(1,182)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:LEU:N	11	1.22
(2,13)	1:113:A:PHE:C	1:114:A:LEU:N	1:114:A:LEU:CA	1:114:A:LEU:C	8	1.21
(1,181)	1:175:A:ILE:C	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	9	1.2
(1,180)	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	1:176:A:VAL:N	2	1.2
(1,44)	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	1:44:A:ILE:N	15	1.2
(2,22)	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1:121:A:PRO:N	14	1.19
(1,66)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:VAL:N	4	1.19
(2,12)	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	1:114:A:LEU:N	1	1.17
(1,67)	1:62:A:VAL:C	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	14	1.17
(1,181)	1:175:A:ILE:C	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	11	1.16
(1,47)	1:44:A:ILE:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	14	1.15
(1,179)	1:174:A:ALA:C	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	2	1.14
(1,48)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:MET:N	10	1.14
(1,47)	1:44:A:ILE:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	3	1.14
(1,45)	1:43:A:THR:C	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	14	1.14
(2,22)	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1:121:A:PRO:N	11	1.13
(2,12)	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	1:114:A:LEU:N	9	1.1
(1,66)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:VAL:N	14	1.1
(1,65)	1:61:A:ARG:C	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	11	1.1
(1,166)	1:168:A:ILE:N	1:168:A:ILE:CA	1:168:A:ILE:C	1:169:A:ARG:N	5	1.08
(1,67)	1:62:A:VAL:C	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	6	1.08
(1,134)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:GLY:N	15	1.07
(1,43)	1:42:A:LEU:C	1:43:A:THR:N	1:43:A:THR:CA	1:43:A:THR:C	15	1.07
(1,143)	1:148:A:VAL:C	1:149:A:THR:N	1:149:A:THR:CA	1:149:A:THR:C	2	1.06
(1,141)	1:147:A:ALA:C	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	5	1.06
(1,66)	1:62:A:VAL:N	1:62:A:VAL:CA	1:62:A:VAL:C	1:63:A:VAL:N	11	1.06
(1,182)	1:176:A:VAL:N	1:176:A:VAL:CA	1:176:A:VAL:C	1:177:A:LEU:N	3	1.05
(1,179)	1:174:A:ALA:C	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	4	1.04
(1,179)	1:174:A:ALA:C	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	11	1.04
(1,67)	1:62:A:VAL:C	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	11	1.04
(1,51)	1:46:A:MET:C	1:47:A:LEU:N	1:47:A:LEU:CA	1:47:A:LEU:C	15	1.04
(2,12)	1:113:A:PHE:N	1:113:A:PHE:CA	1:113:A:PHE:C	1:114:A:LEU:N	2	1.03
(1,180)	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	1:176:A:VAL:N	7	1.03
(2,22)	1:120:A:LEU:N	1:120:A:LEU:CA	1:120:A:LEU:C	1:121:A:PRO:N	4	1.02
(1,180)	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	1:176:A:VAL:N	15	1.02
(1,79)	1:68:A:LEU:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	11	1.02
(1,78)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:LEU:N	11	1.02
(1,67)	1:62:A:VAL:C	1:63:A:VAL:N	1:63:A:VAL:CA	1:63:A:VAL:C	15	1.02
(1,46)	1:44:A:ILE:N	1:44:A:ILE:CA	1:44:A:ILE:C	1:45:A:SER:N	2	1.02
(1,179)	1:174:A:ALA:C	1:175:A:ILE:N	1:175:A:ILE:CA	1:175:A:ILE:C	15	1.01
(1,175)	1:172:A:THR:C	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	4	1.01
(1,175)	1:172:A:THR:C	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	8	1.01
(1,175)	1:172:A:THR:C	1:173:A:GLY:N	1:173:A:GLY:CA	1:173:A:GLY:C	10	1.01
(2,15)	1:114:A:LEU:C	1:115:A:TRP:N	1:115:A:TRP:CA	1:115:A:TRP:C	15	1.0
(1,142)	1:148:A:VAL:N	1:148:A:VAL:CA	1:148:A:VAL:C	1:149:A:THR:N	6	1.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,134)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:GLY:N	12	1.0