



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:21 AM UTC

PDB ID : 2MMN / pdb_00002mmn
BMRB ID : 6282
Title : Solution Structure of the Reduced Thioredoxin from Plasmodium falciparum
Authors : Munte, C.; Kalbitzer, H.; Schirmer, R.
Deposited on : 2014-03-16

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

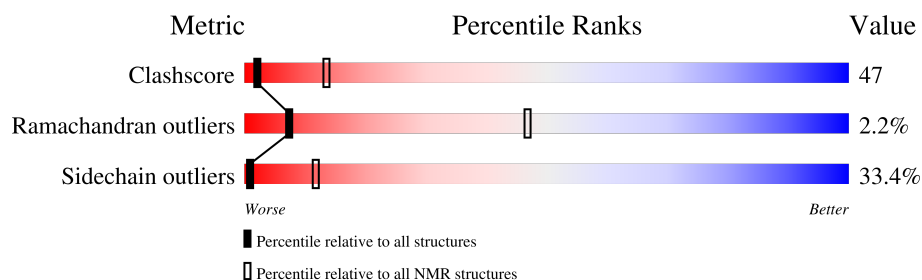
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	104	28% 59% 12% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:104 (103)	0.37	1

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

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

The models can be grouped into 2 clusters and 4 single-model clusters were found.

Cluster number	Models
1	6, 8, 10
2	1, 2, 3
Single-model clusters	4; 5; 7; 9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1631 atoms, of which 813 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms							Trace
1	A	104	Total	C	H	N	O	S		0
			1631	524	813	125	164	5		

There are 2 discrepancies between the modelled and reference sequences:

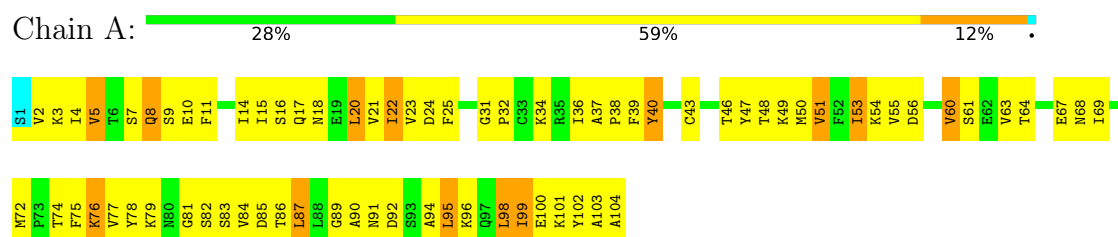
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q7KQL8
A	9	SER	ALA	conflict	UNP Q7KQL8

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Thioredoxin

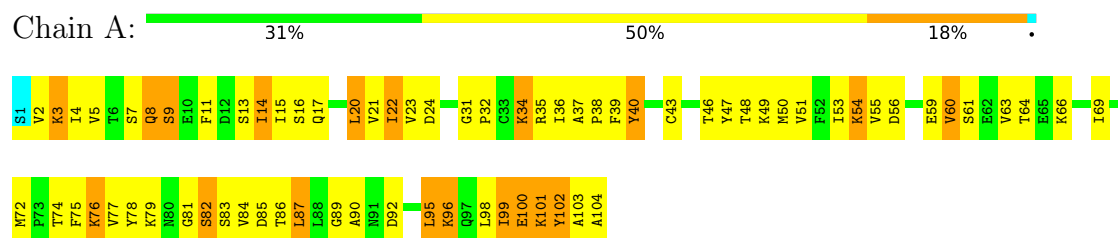


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

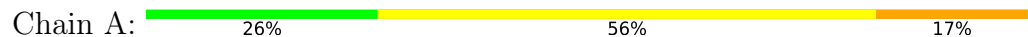
4.2.1 Score per residue for model 1 (medoid)

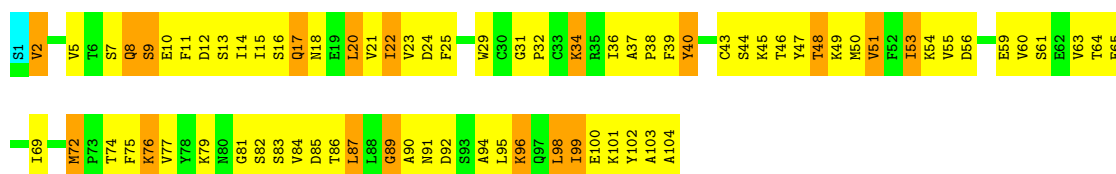
- Molecule 1: Thioredoxin



4.2.2 Score per residue for model 2

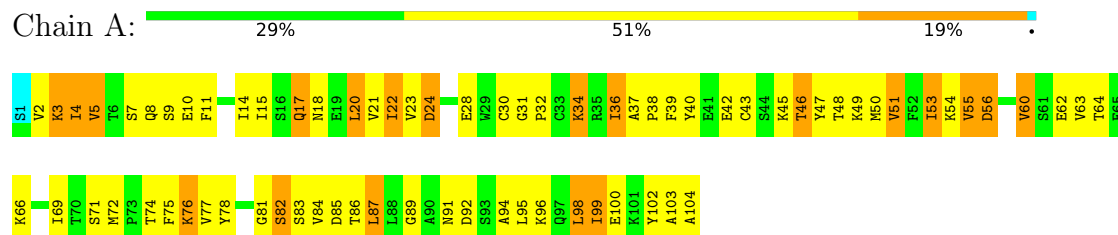
- Molecule 1: Thioredoxin





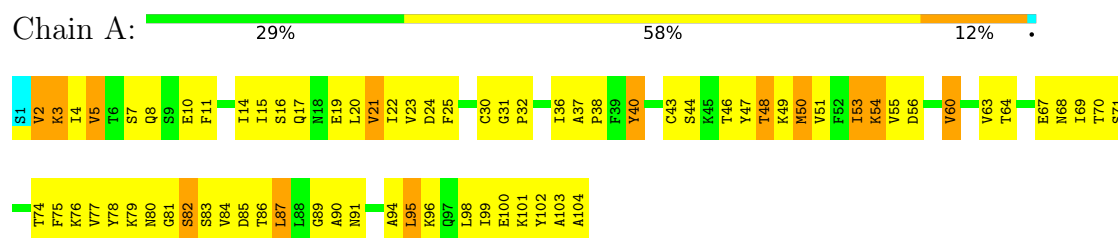
4.2.3 Score per residue for model 3

- Molecule 1: Thioredoxin



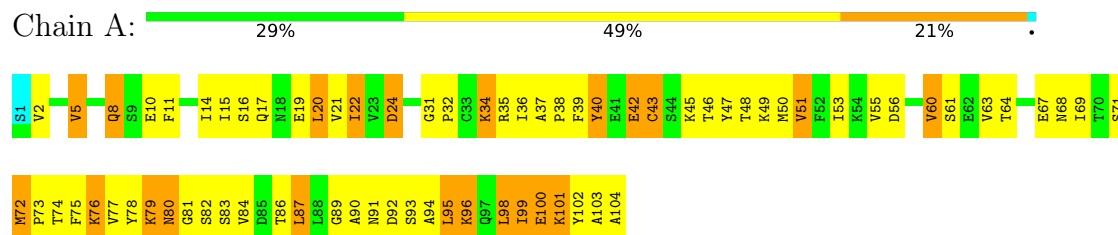
4.2.4 Score per residue for model 4

- Molecule 1: Thioredoxin



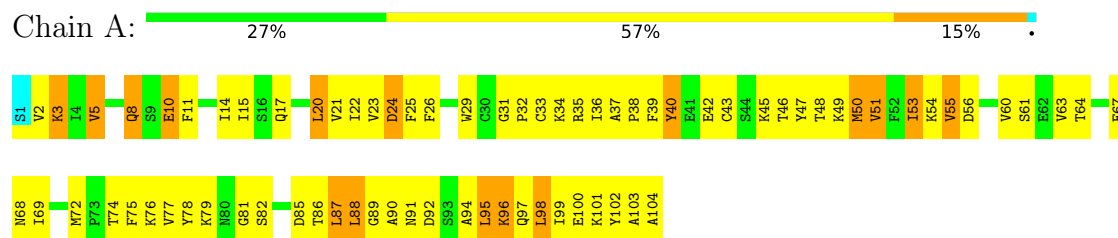
4.2.5 Score per residue for model 5

- Molecule 1: Thioredoxin



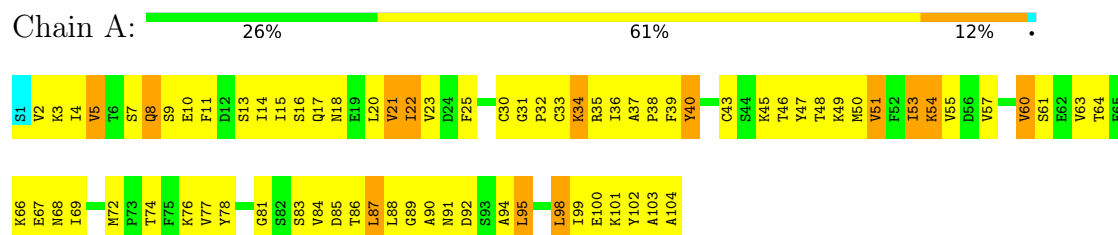
4.2.6 Score per residue for model 6

- Molecule 1: Thioredoxin



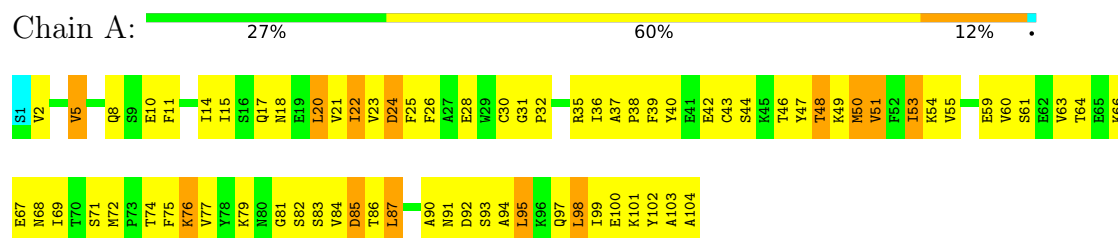
4.2.7 Score per residue for model 7

- Molecule 1: Thioredoxin



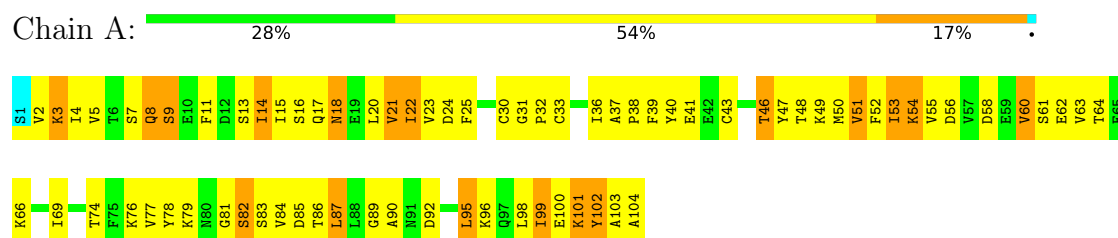
4.2.8 Score per residue for model 8

- Molecule 1: Thioredoxin



4.2.9 Score per residue for model 9

- Molecule 1: Thioredoxin



4.2.10 Score per residue for model 10

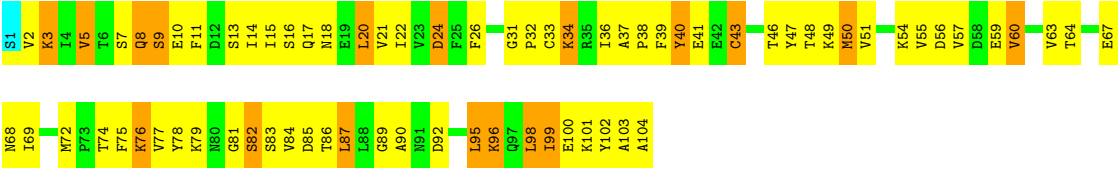
● Molecule 1: Thioredoxin

Chain A:

29%

53%

17%



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1266
Number of shifts mapped to atoms	1265
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	812	809	809	77±8
All	All	8120	8090	8090	769

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 47.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD21	1:A:102:TYR:HB3	0.91	1.42	10	8
1:A:11:PHE:CE2	1:A:63:VAL:HG13	0.91	1.99	7	10
1:A:50:MET:HE1	1:A:102:TYR:HB2	0.91	1.42	5	2
1:A:21:VAL:HG12	1:A:53:ILE:HD11	0.90	1.42	9	2
1:A:21:VAL:HG13	1:A:51:VAL:HG12	0.90	1.44	3	4
1:A:76:LYS:HD2	1:A:86:THR:HG22	0.89	1.45	2	2
1:A:5:VAL:CG1	1:A:55:VAL:HG22	0.85	2.01	1	5
1:A:20:LEU:HD12	1:A:50:MET:CE	0.82	2.03	5	1
1:A:3:LYS:O	1:A:54:LYS:N	0.82	2.12	10	7
1:A:20:LEU:HA	1:A:78:TYR:O	0.81	1.75	5	4
1:A:20:LEU:HD23	1:A:50:MET:HE3	0.80	1.51	4	1
1:A:11:PHE:CD1	1:A:55:VAL:HG21	0.80	2.12	8	8
1:A:77:VAL:O	1:A:84:VAL:HG12	0.79	1.78	4	9
1:A:2:VAL:HG12	1:A:54:LYS:CE	0.79	2.07	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:HG11	1:A:63:VAL:HG11	0.79	1.53	3	9
1:A:72:MET:O	1:A:72:MET:HE2	0.78	1.79	2	1
1:A:47:TYR:CD2	1:A:99:ILE:HG12	0.77	2.14	8	4
1:A:36:ILE:HD13	1:A:90:ALA:C	0.77	2.05	4	2
1:A:23:VAL:HG22	1:A:53:ILE:HG13	0.76	1.57	1	1
1:A:32:PRO:O	1:A:36:ILE:HG22	0.76	1.79	9	10
1:A:99:ILE:O	1:A:103:ALA:HB3	0.75	1.80	9	10
1:A:21:VAL:HG13	1:A:51:VAL:CG1	0.75	2.12	2	4
1:A:20:LEU:HD23	1:A:50:MET:CE	0.74	2.10	4	5
1:A:15:ILE:HG22	1:A:81:GLY:HA2	0.74	1.58	1	6
1:A:5:VAL:HG11	1:A:14:ILE:CD1	0.74	2.12	6	3
1:A:64:THR:HG23	1:A:69:ILE:HB	0.73	1.60	7	10
1:A:23:VAL:HG22	1:A:53:ILE:CG1	0.73	2.13	1	1
1:A:20:LEU:HB2	1:A:50:MET:HE2	0.73	1.61	5	1
1:A:31:GLY:N	1:A:32:PRO:HD2	0.72	2.00	4	10
1:A:76:LYS:HG2	1:A:86:THR:HG22	0.72	1.61	6	7
1:A:76:LYS:CG	1:A:86:THR:HG22	0.72	2.15	10	7
1:A:2:VAL:HG21	1:A:40:TYR:CD2	0.72	2.18	10	1
1:A:47:TYR:CE2	1:A:99:ILE:CG2	0.71	2.74	9	10
1:A:20:LEU:HD21	1:A:102:TYR:CB	0.71	2.15	9	4
1:A:14:ILE:HG22	1:A:21:VAL:HG11	0.71	1.61	4	8
1:A:22:ILE:HD12	1:A:77:VAL:HG22	0.71	1.59	3	4
1:A:5:VAL:HG13	1:A:55:VAL:HG22	0.71	1.61	8	6
1:A:22:ILE:HD12	1:A:77:VAL:CG2	0.69	2.18	3	3
1:A:2:VAL:HG12	1:A:54:LYS:HE3	0.69	1.65	4	1
1:A:22:ILE:HG22	1:A:50:MET:HG2	0.68	1.66	5	4
1:A:5:VAL:HG11	1:A:14:ILE:HD11	0.67	1.66	6	2
1:A:3:LYS:HB3	1:A:53:ILE:HG22	0.67	1.66	9	2
1:A:20:LEU:HD23	1:A:50:MET:SD	0.67	2.29	4	2
1:A:85:ASP:OD2	1:A:98:LEU:HD12	0.67	1.89	3	3
1:A:22:ILE:HD13	1:A:99:ILE:HG12	0.67	1.67	5	2
1:A:5:VAL:HG13	1:A:55:VAL:CG2	0.67	2.20	7	2
1:A:23:VAL:HG13	1:A:25:PHE:CE1	0.67	2.25	4	4
1:A:20:LEU:HD12	1:A:78:TYR:O	0.66	1.90	4	6
1:A:50:MET:HE1	1:A:102:TYR:C	0.66	2.16	3	4
1:A:44:SER:O	1:A:48:THR:HG22	0.65	1.92	4	3
1:A:11:PHE:O	1:A:15:ILE:HG12	0.65	1.91	10	10
1:A:20:LEU:HG	1:A:50:MET:HE3	0.64	1.70	7	1
1:A:18:ASN:OD1	1:A:21:VAL:HG22	0.64	1.92	9	1
1:A:37:ALA:O	1:A:41:GLU:HG3	0.64	1.93	9	1
1:A:50:MET:SD	1:A:103:ALA:HB2	0.63	2.33	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LYS:CD	1:A:86:THR:HG22	0.63	2.22	2	6
1:A:10:GLU:O	1:A:14:ILE:HD12	0.63	1.93	5	8
1:A:2:VAL:HG12	1:A:54:LYS:HD2	0.63	1.70	2	3
1:A:95:LEU:O	1:A:99:ILE:HG22	0.62	1.94	7	4
1:A:96:LYS:O	1:A:100:GLU:HB2	0.62	1.93	1	6
1:A:20:LEU:HD12	1:A:50:MET:HE3	0.62	1.70	5	1
1:A:20:LEU:HD23	1:A:50:MET:HE2	0.62	1.71	1	2
1:A:37:ALA:HB3	1:A:38:PRO:HD3	0.62	1.70	9	5
1:A:50:MET:HE1	1:A:102:TYR:CB	0.62	2.20	5	2
1:A:47:TYR:CE2	1:A:99:ILE:HG23	0.62	2.29	2	5
1:A:50:MET:HE2	1:A:77:VAL:HG13	0.62	1.70	7	1
1:A:47:TYR:CD2	1:A:99:ILE:HD12	0.62	2.29	2	3
1:A:24:ASP:HB2	1:A:75:PHE:CE1	0.62	2.29	10	5
1:A:60:VAL:HB	1:A:63:VAL:HG23	0.61	1.71	3	7
1:A:72:MET:HE3	1:A:73:PRO:HD3	0.61	1.70	5	1
1:A:5:VAL:HG22	1:A:55:VAL:HG22	0.61	1.71	4	2
1:A:53:ILE:N	1:A:53:ILE:HD13	0.61	2.10	8	2
1:A:36:ILE:HB	1:A:90:ALA:HB1	0.61	1.72	9	6
1:A:100:GLU:CA	1:A:104:ALA:HB3	0.60	2.26	3	7
1:A:20:LEU:HG	1:A:50:MET:HE2	0.60	1.72	3	4
1:A:21:VAL:CG1	1:A:53:ILE:HD11	0.60	2.21	9	2
1:A:47:TYR:CG	1:A:99:ILE:HD12	0.60	2.32	2	1
1:A:22:ILE:HG21	1:A:52:PHE:CE1	0.60	2.32	9	1
1:A:39:PHE:CE2	1:A:95:LEU:HD23	0.60	2.31	10	3
1:A:39:PHE:CE2	1:A:92:ASP:O	0.59	2.55	1	7
1:A:39:PHE:CD2	1:A:95:LEU:HD23	0.59	2.32	10	5
1:A:20:LEU:CG	1:A:50:MET:HE2	0.59	2.27	3	4
1:A:47:TYR:CD2	1:A:99:ILE:CG1	0.59	2.85	7	4
1:A:99:ILE:HD13	1:A:103:ALA:HB3	0.59	1.73	2	3
1:A:33:CYS:O	1:A:37:ALA:HB2	0.59	1.98	6	4
1:A:37:ALA:N	1:A:38:PRO:HD2	0.59	2.12	8	4
1:A:50:MET:CE	1:A:102:TYR:HB2	0.59	2.28	7	1
1:A:18:ASN:HB2	1:A:21:VAL:HG22	0.58	1.75	8	3
1:A:99:ILE:HD13	1:A:103:ALA:CB	0.58	2.28	10	3
1:A:20:LEU:HG	1:A:50:MET:CE	0.58	2.28	7	3
1:A:98:LEU:HD12	1:A:98:LEU:O	0.58	1.98	6	1
1:A:77:VAL:HG21	1:A:102:TYR:CE2	0.58	2.34	8	1
1:A:87:LEU:HB3	1:A:98:LEU:HD13	0.57	1.75	8	2
1:A:20:LEU:N	1:A:20:LEU:HD23	0.57	2.13	5	1
1:A:77:VAL:HG21	1:A:102:TYR:CD2	0.57	2.35	8	3
1:A:20:LEU:CD2	1:A:50:MET:HE2	0.57	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ASP:OD2	1:A:98:LEU:HD13	0.57	1.99	6	1
1:A:8:GLN:NE2	1:A:63:VAL:HG22	0.56	2.15	7	6
1:A:40:TYR:HA	1:A:43:CYS:SG	0.56	2.39	5	3
1:A:47:TYR:CE2	1:A:99:ILE:HG21	0.56	2.36	8	5
1:A:20:LEU:HD21	1:A:102:TYR:HB2	0.56	1.77	9	1
1:A:43:CYS:O	1:A:47:TYR:HB2	0.56	2.01	2	4
1:A:31:GLY:N	1:A:32:PRO:CD	0.55	2.69	4	10
1:A:18:ASN:OD1	1:A:21:VAL:CG2	0.55	2.55	9	1
1:A:100:GLU:HA	1:A:104:ALA:HB3	0.55	1.78	9	7
1:A:87:LEU:CB	1:A:98:LEU:HD13	0.55	2.32	8	1
1:A:14:ILE:HG21	1:A:53:ILE:HG21	0.55	1.78	7	4
1:A:18:ASN:OD1	1:A:51:VAL:HG21	0.55	2.02	9	1
1:A:5:VAL:CG1	1:A:55:VAL:HG23	0.55	2.32	3	2
1:A:46:THR:CG2	1:A:47:TYR:CD1	0.55	2.90	9	1
1:A:23:VAL:HG23	1:A:53:ILE:O	0.54	2.03	7	4
1:A:102:TYR:N	1:A:102:TYR:CD1	0.54	2.75	1	2
1:A:15:ILE:O	1:A:81:GLY:HA2	0.54	2.02	4	6
1:A:19:GLU:O	1:A:80:ASN:N	0.54	2.40	5	1
1:A:85:ASP:CB	1:A:102:TYR:OH	0.54	2.56	8	3
1:A:47:TYR:CD2	1:A:99:ILE:HG23	0.54	2.38	9	1
1:A:87:LEU:HD12	1:A:87:LEU:C	0.53	2.29	6	9
1:A:14:ILE:HG22	1:A:21:VAL:CG1	0.53	2.33	4	1
1:A:55:VAL:CG1	1:A:63:VAL:HG11	0.53	2.28	3	2
1:A:20:LEU:HB3	1:A:50:MET:SD	0.53	2.43	9	1
1:A:47:TYR:CE1	1:A:104:ALA:HB2	0.53	2.38	9	1
1:A:20:LEU:HD11	1:A:77:VAL:HG12	0.53	1.80	9	2
1:A:39:PHE:CE2	1:A:43:CYS:SG	0.53	3.02	6	7
1:A:43:CYS:O	1:A:47:TYR:CD2	0.53	2.61	1	8
1:A:77:VAL:C	1:A:84:VAL:HG12	0.52	2.29	9	4
1:A:3:LYS:O	1:A:54:LYS:HE2	0.52	2.04	4	1
1:A:87:LEU:HD11	1:A:89:GLY:O	0.52	2.05	2	1
1:A:17:GLN:HA	1:A:17:GLN:OE1	0.52	2.04	8	2
1:A:5:VAL:HG13	1:A:55:VAL:HG23	0.51	1.82	3	2
1:A:100:GLU:HA	1:A:104:ALA:CB	0.51	2.36	3	7
1:A:47:TYR:CD2	1:A:99:ILE:CG2	0.51	2.93	9	2
1:A:98:LEU:HD12	1:A:98:LEU:C	0.51	2.31	6	1
1:A:50:MET:HE2	1:A:50:MET:CA	0.51	2.36	9	1
1:A:4:ILE:HG23	1:A:4:ILE:O	0.51	2.04	7	5
1:A:5:VAL:HG23	1:A:10:GLU:CG	0.51	2.36	2	1
1:A:2:VAL:HG11	1:A:54:LYS:HD2	0.50	1.82	1	1
1:A:23:VAL:HA	1:A:53:ILE:O	0.50	2.05	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HG12	1:A:90:ALA:HB1	0.50	1.84	8	3
1:A:36:ILE:O	1:A:40:TYR:HB2	0.50	2.06	10	7
1:A:36:ILE:CB	1:A:90:ALA:HB1	0.50	2.37	6	6
1:A:77:VAL:HG21	1:A:102:TYR:HD2	0.50	1.65	9	1
1:A:43:CYS:HB3	1:A:47:TYR:CD2	0.50	2.41	3	3
1:A:91:ASN:HB2	1:A:94:ALA:HB3	0.50	1.83	6	7
1:A:14:ILE:O	1:A:21:VAL:HG21	0.50	2.07	3	1
1:A:11:PHE:CD2	1:A:63:VAL:HG13	0.50	2.41	2	7
1:A:24:ASP:CB	1:A:75:PHE:CE1	0.50	2.95	4	3
1:A:36:ILE:CG1	1:A:90:ALA:HB1	0.50	2.37	4	2
1:A:2:VAL:HG11	1:A:54:LYS:CD	0.50	2.37	6	1
1:A:20:LEU:CD2	1:A:50:MET:CE	0.49	2.90	1	1
1:A:20:LEU:HD12	1:A:50:MET:HE2	0.49	1.82	5	1
1:A:18:ASN:CG	1:A:51:VAL:HG21	0.49	2.33	9	1
1:A:50:MET:HE2	1:A:50:MET:HA	0.49	1.84	9	1
1:A:5:VAL:HG23	1:A:10:GLU:HG2	0.49	1.85	2	1
1:A:5:VAL:CG1	1:A:55:VAL:CG2	0.49	2.91	9	3
1:A:20:LEU:CD2	1:A:50:MET:HE3	0.48	2.32	4	2
1:A:31:GLY:H	1:A:32:PRO:HD2	0.48	1.67	8	6
1:A:37:ALA:N	1:A:38:PRO:CD	0.48	2.76	1	6
1:A:100:GLU:O	1:A:104:ALA:CA	0.48	2.62	2	4
1:A:99:ILE:O	1:A:103:ALA:CB	0.48	2.58	9	5
1:A:22:ILE:CG2	1:A:52:PHE:CD1	0.48	2.97	9	1
1:A:46:THR:CG2	1:A:47:TYR:CE1	0.48	2.97	9	1
1:A:42:GLU:HG3	1:A:43:CYS:N	0.48	2.22	5	4
1:A:23:VAL:CG1	1:A:25:PHE:CE1	0.47	2.96	2	1
1:A:20:LEU:CB	1:A:50:MET:SD	0.47	3.02	9	1
1:A:20:LEU:CG	1:A:50:MET:SD	0.47	3.02	9	1
1:A:11:PHE:HD1	1:A:55:VAL:HG21	0.47	1.64	8	2
1:A:21:VAL:HG22	1:A:51:VAL:HG23	0.47	1.84	5	1
1:A:101:LYS:NZ	1:A:102:TYR:CE1	0.47	2.82	5	1
1:A:22:ILE:CD1	1:A:77:VAL:HG22	0.47	2.40	9	1
1:A:9:SER:O	1:A:13:SER:N	0.47	2.47	9	5
1:A:77:VAL:CG2	1:A:98:LEU:HD11	0.47	2.40	6	1
1:A:85:ASP:HB2	1:A:102:TYR:OH	0.47	2.09	2	1
1:A:32:PRO:O	1:A:36:ILE:N	0.47	2.46	5	7
1:A:68:ASN:O	1:A:68:ASN:CG	0.47	2.58	8	1
1:A:24:ASP:OD1	1:A:24:ASP:N	0.47	2.47	2	2
1:A:20:LEU:CA	1:A:78:TYR:O	0.47	2.58	5	1
1:A:20:LEU:HD12	1:A:78:TYR:C	0.47	2.35	9	1
1:A:99:ILE:CD1	1:A:103:ALA:CB	0.46	2.92	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLU:OE1	1:A:28:GLU:N	0.46	2.46	3	1
1:A:53:ILE:HA	1:A:54:LYS:HE2	0.46	1.87	4	1
1:A:34:LYS:O	1:A:38:PRO:HD3	0.46	2.10	3	5
1:A:100:GLU:O	1:A:104:ALA:HA	0.46	2.10	7	2
1:A:43:CYS:SG	1:A:95:LEU:HD21	0.46	2.51	5	2
1:A:38:PRO:O	1:A:41:GLU:HG2	0.46	2.11	10	1
1:A:2:VAL:CG1	1:A:54:LYS:HE3	0.46	2.40	4	1
1:A:22:ILE:HG22	1:A:50:MET:HG3	0.45	1.87	9	1
1:A:21:VAL:HG22	1:A:51:VAL:CG2	0.45	2.41	5	1
1:A:47:TYR:HB3	1:A:103:ALA:HB1	0.45	1.88	5	1
1:A:56:ASP:O	1:A:60:VAL:HG23	0.45	2.11	3	1
1:A:68:ASN:OD1	1:A:68:ASN:O	0.45	2.34	7	4
1:A:68:ASN:O	1:A:70:THR:HG23	0.45	2.11	4	1
1:A:14:ILE:O	1:A:18:ASN:ND2	0.45	2.50	9	1
1:A:67:GLU:O	1:A:68:ASN:ND2	0.45	2.50	8	6
1:A:47:TYR:CG	1:A:99:ILE:CG1	0.45	3.00	6	3
1:A:68:ASN:O	1:A:68:ASN:OD1	0.45	2.35	8	2
1:A:26:PHE:CZ	1:A:54:LYS:CE	0.45	3.00	8	2
1:A:24:ASP:OD1	1:A:54:LYS:HA	0.45	2.11	4	1
1:A:72:MET:HE3	1:A:73:PRO:CD	0.45	2.42	5	1
1:A:47:TYR:CD1	1:A:104:ALA:HB2	0.45	2.47	9	1
1:A:77:VAL:HG23	1:A:98:LEU:HD21	0.45	1.89	10	1
1:A:78:TYR:HA	1:A:82:SER:O	0.44	2.12	3	6
1:A:57:VAL:HG12	1:A:64:THR:OG1	0.44	2.12	7	2
1:A:47:TYR:CG	1:A:99:ILE:HG12	0.44	2.46	6	3
1:A:22:ILE:HD12	1:A:23:VAL:N	0.44	2.27	8	1
1:A:2:VAL:HG21	1:A:40:TYR:HD2	0.44	1.70	10	1
1:A:20:LEU:CG	1:A:50:MET:HE3	0.44	2.39	7	1
1:A:100:GLU:O	1:A:104:ALA:C	0.44	2.60	3	5
1:A:43:CYS:HB3	1:A:47:TYR:CE2	0.44	2.48	3	2
1:A:19:GLU:C	1:A:20:LEU:HD23	0.44	2.38	5	1
1:A:95:LEU:HD11	1:A:99:ILE:CG1	0.44	2.43	9	1
1:A:100:GLU:O	1:A:104:ALA:N	0.44	2.51	4	5
1:A:101:LYS:HB3	1:A:102:TYR:CD1	0.44	2.48	9	2
1:A:87:LEU:HD12	1:A:88:LEU:N	0.44	2.28	7	2
1:A:43:CYS:O	1:A:47:TYR:CG	0.43	2.71	3	1
1:A:21:VAL:O	1:A:78:TYR:N	0.43	2.42	1	3
1:A:34:LYS:O	1:A:38:PRO:CD	0.43	2.66	2	1
1:A:39:PHE:CE1	1:A:42:GLU:CD	0.43	2.97	5	2
1:A:53:ILE:N	1:A:53:ILE:CD1	0.43	2.79	8	2
1:A:26:PHE:CE1	1:A:56:ASP:OD1	0.43	2.72	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ILE:CD1	1:A:103:ALA:HB3	0.43	2.43	2	1
1:A:53:ILE:CA	1:A:54:LYS:HE2	0.43	2.43	4	1
1:A:3:LYS:N	1:A:54:LYS:HE3	0.43	2.29	4	1
1:A:96:LYS:HG3	1:A:97:GLN:N	0.43	2.28	6	1
1:A:24:ASP:HB3	1:A:75:PHE:CE1	0.42	2.48	1	1
1:A:13:SER:OG	1:A:17:GLN:NE2	0.42	2.52	2	1
1:A:29:TRP:O	1:A:29:TRP:CE3	0.42	2.72	6	2
1:A:46:THR:HG22	1:A:47:TYR:CD1	0.42	2.49	3	2
1:A:33:CYS:O	1:A:37:ALA:CB	0.42	2.67	6	1
1:A:50:MET:CE	1:A:77:VAL:CG1	0.42	2.97	7	1
1:A:21:VAL:HG13	1:A:51:VAL:HG23	0.42	1.90	9	1
1:A:43:CYS:HA	1:A:47:TYR:CE2	0.42	2.49	1	1
1:A:96:LYS:HD3	1:A:96:LYS:C	0.42	2.40	1	1
1:A:7:SER:OG	1:A:10:GLU:CB	0.42	2.68	3	1
1:A:20:LEU:O	1:A:51:VAL:HG23	0.42	2.15	7	1
1:A:50:MET:HE2	1:A:103:ALA:HA	0.42	1.92	4	1
1:A:101:LYS:HE2	1:A:102:TYR:CE1	0.42	2.49	5	1
1:A:2:VAL:CG1	1:A:54:LYS:HD2	0.42	2.45	3	2
1:A:85:ASP:CG	1:A:102:TYR:CZ	0.42	2.98	1	2
1:A:8:GLN:CD	1:A:8:GLN:C	0.42	2.87	10	3
1:A:23:VAL:CG2	1:A:53:ILE:CD1	0.42	2.98	3	2
1:A:2:VAL:HG12	1:A:54:LYS:NZ	0.42	2.30	4	1
1:A:20:LEU:CD1	1:A:77:VAL:HG12	0.41	2.45	1	1
1:A:24:ASP:OD1	1:A:26:PHE:HB3	0.41	2.14	10	1
1:A:24:ASP:OD1	1:A:54:LYS:CG	0.41	2.68	1	1
1:A:53:ILE:C	1:A:54:LYS:HE2	0.41	2.40	4	1
1:A:67:GLU:HG3	1:A:78:TYR:OH	0.41	2.15	4	1
1:A:29:TRP:O	1:A:29:TRP:HE3	0.41	1.98	6	1
1:A:11:PHE:CZ	1:A:67:GLU:OE2	0.41	2.74	8	1
1:A:76:LYS:HD3	1:A:86:THR:CG2	0.41	2.45	9	1
1:A:76:LYS:HG2	1:A:78:TYR:CE1	0.41	2.50	9	1
1:A:26:PHE:CZ	1:A:54:LYS:HE3	0.41	2.50	10	1
1:A:98:LEU:O	1:A:102:TYR:CD1	0.41	2.74	10	1
1:A:87:LEU:CD2	1:A:98:LEU:HD22	0.41	2.45	7	1
1:A:20:LEU:HB3	1:A:50:MET:HE1	0.41	1.93	9	1
1:A:39:PHE:CD1	1:A:92:ASP:HB2	0.41	2.51	10	1
1:A:43:CYS:CB	1:A:47:TYR:CD2	0.41	3.04	10	2
1:A:26:PHE:CZ	1:A:56:ASP:OD2	0.41	2.74	10	1
1:A:15:ILE:HG22	1:A:81:GLY:CA	0.41	2.39	1	1
1:A:19:GLU:O	1:A:79:LYS:HA	0.41	2.16	5	1
1:A:20:LEU:N	1:A:20:LEU:CD2	0.41	2.82	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:VAL:HG22	1:A:55:VAL:CG2	0.41	2.46	6	1
1:A:96:LYS:O	1:A:100:GLU:CB	0.41	2.68	9	1
1:A:24:ASP:HB2	1:A:75:PHE:CD1	0.41	2.51	10	2
1:A:87:LEU:C	1:A:87:LEU:CD1	0.41	2.94	6	1
1:A:11:PHE:CE1	1:A:25:PHE:CE1	0.41	3.09	7	1
1:A:21:VAL:N	1:A:78:TYR:O	0.40	2.48	9	1
1:A:26:PHE:CE1	1:A:56:ASP:CG	0.40	2.99	10	1
1:A:94:ALA:O	1:A:97:GLN:HG2	0.40	2.16	8	1
1:A:95:LEU:O	1:A:99:ILE:HB	0.40	2.16	9	1
1:A:24:ASP:OD1	1:A:54:LYS:HG3	0.40	2.17	1	2
1:A:43:CYS:CB	1:A:47:TYR:HD2	0.40	2.30	5	1
1:A:22:ILE:CG2	1:A:52:PHE:CE1	0.40	3.04	9	1
1:A:22:ILE:HD13	1:A:77:VAL:HG22	0.40	1.93	9	1
1:A:18:ASN:HB2	1:A:21:VAL:CG2	0.40	2.47	3	2
1:A:87:LEU:C	1:A:87:LEU:HD12	0.40	2.41	4	1
1:A:56:ASP:OD1	1:A:59:GLU:CB	0.40	2.70	1	1
1:A:99:ILE:O	1:A:99:ILE:HD13	0.40	2.16	2	1
1:A:62:GLU:O	1:A:66:LYS:CG	0.40	2.70	3	1
1:A:39:PHE:CD1	1:A:92:ASP:HB3	0.40	2.51	5	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/104 (98%)	96±1 (94±1%)	4±1 (4±1%)	2±0 (2±0%)	7	47
All	All	1020/1040 (98%)	959 (94%)	39 (4%)	22 (2%)	7	47

All 3 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	48	THR	10
1	A	89	GLY	9
1	A	2	VAL	3

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	94/95 (99%)	63±2 (67±2%)	31±2 (33±2%)	1	12
All	All	940/950 (99%)	626 (67%)	314 (33%)	1	12

All 61 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	8	GLN	10
1	A	22	ILE	10
1	A	46	THR	10
1	A	49	LYS	10
1	A	51	VAL	10
1	A	60	VAL	10
1	A	74	THR	10
1	A	87	LEU	10
1	A	95	LEU	10
1	A	98	LEU	10
1	A	17	GLN	9
1	A	40	TYR	9
1	A	83	SER	9
1	A	101	LYS	9
1	A	72	MET	8
1	A	79	LYS	8
1	A	82	SER	8
1	A	53	ILE	8
1	A	16	SER	7
1	A	20	LEU	7
1	A	34	LYS	7
1	A	61	SER	7
1	A	5	VAL	7
1	A	3	LYS	6
1	A	7	SER	6
1	A	76	LYS	6
1	A	96	LYS	6
1	A	99	ILE	6
1	A	56	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	9	SER	5
1	A	35	ARG	5
1	A	45	LYS	5
1	A	24	ASP	5
1	A	30	CYS	5
1	A	54	LYS	4
1	A	66	LYS	4
1	A	71	SER	4
1	A	50	MET	4
1	A	59	GLU	3
1	A	21	VAL	3
1	A	14	ILE	2
1	A	100	GLU	2
1	A	102	TYR	2
1	A	55	VAL	2
1	A	80	ASN	2
1	A	43	CYS	2
1	A	93	SER	2
1	A	12	ASP	1
1	A	65	GLU	1
1	A	4	ILE	1
1	A	36	ILE	1
1	A	2	VAL	1
1	A	19	GLU	1
1	A	42	GLU	1
1	A	10	GLU	1
1	A	88	LEU	1
1	A	28	GLU	1
1	A	85	ASP	1
1	A	18	ASN	1
1	A	58	ASP	1
1	A	62	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1266
Number of shifts mapped to atoms	1265
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	SER	H	8.26	.	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	102	-0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	99	0.28 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	93	-0.05 ± 0.08	None needed (< 0.5 ppm)
^{15}N	100	0.25 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1250 atoms were assigned a chemical shift out of a possible 1384. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	496/512 (97%)	204/206 (99%)	193/206 (94%)	99/100 (99%)
Sidechain	706/764 (92%)	486/497 (98%)	213/247 (86%)	7/20 (35%)
Aromatic	48/108 (44%)	47/52 (90%)	0/55 (0%)	1/1 (100%)
Overall	1250/1384 (90%)	737/755 (98%)	406/508 (80%)	107/121 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1258 atoms were assigned a chemical shift out of a possible 1392. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	501/517 (97%)	206/208 (99%)	195/208 (94%)	100/101 (99%)
Sidechain	709/767 (92%)	488/499 (98%)	214/248 (86%)	7/20 (35%)
Aromatic	48/108 (44%)	47/52 (90%)	0/55 (0%)	1/1 (100%)
Overall	1258/1392 (90%)	741/759 (98%)	409/511 (80%)	108/122 (89%)

7.1.4 Statistically unusual chemical shifts [i](#)

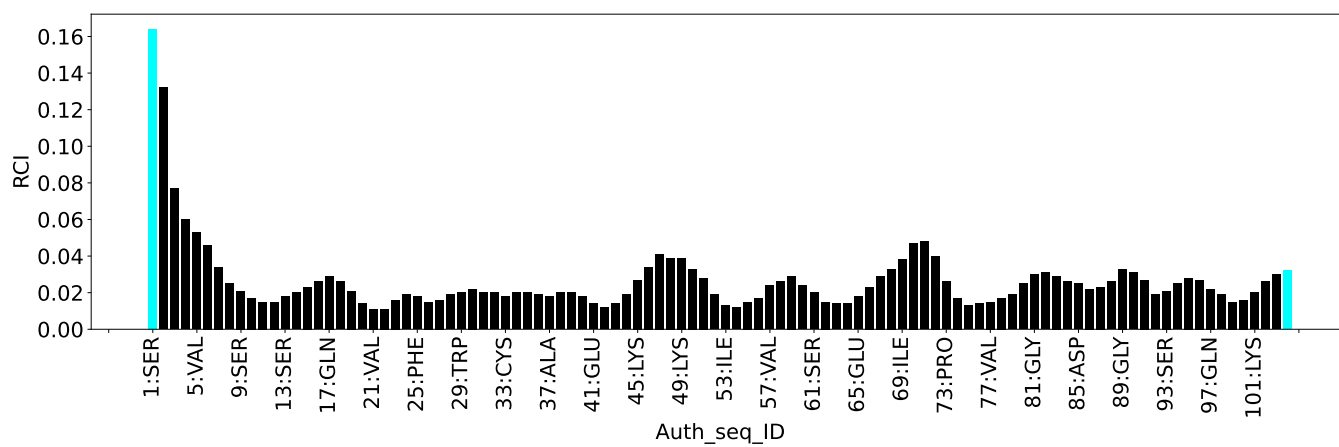
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	101	LYS	CE	13.78	37.57 – 46.21	-32.5
1	A	101	LYS	CD	20.62	23.50 – 34.42	-7.6

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	2962
Intra-residue ($ i-j =0$)	725
Sequential ($ i-j =1$)	695
Medium range ($ i-j >1$ and $ i-j <5$)	562
Long range ($ i-j \geq 5$)	980
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	180
Number of unmapped restraints	0
Number of restraints per residue	30.2
Number of long range restraints per residue ¹	9.4

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)	54.4	0.2
0.2-0.5 (Medium)	69.3	0.5
>0.5 (Large)	31.4	1.54

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)	35.5	9.78
10.0-20.0 (Medium)	0.6	10.7
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

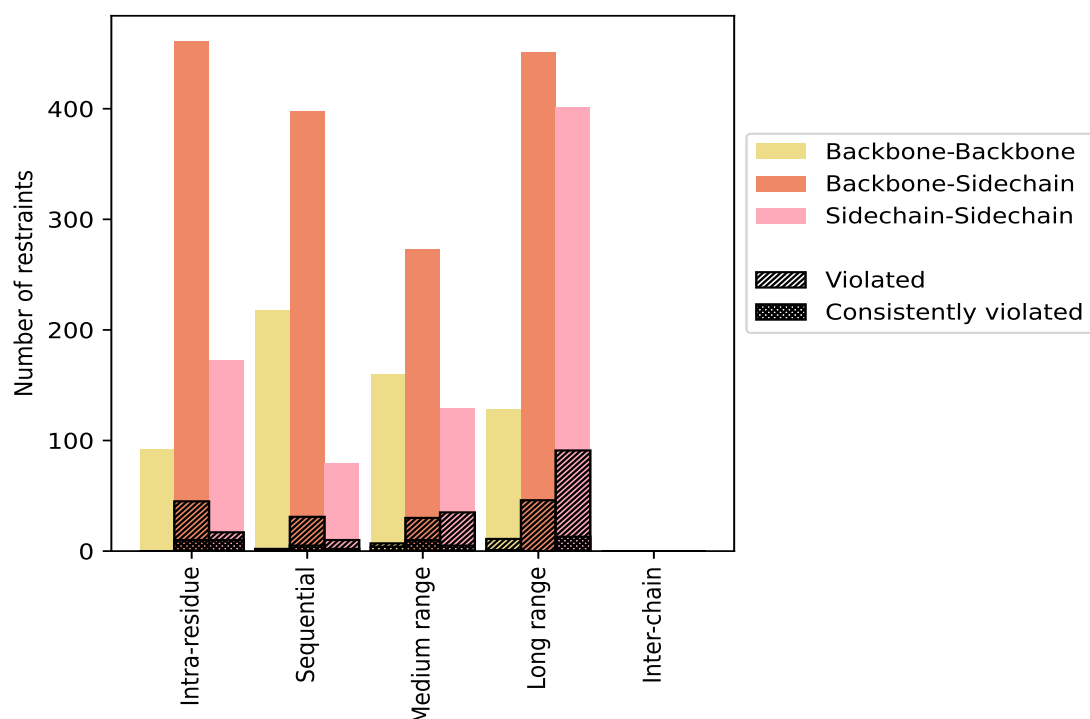
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	725	24.5	62	8.6	2.1	20	2.8	0.7
Backbone-Backbone	92	3.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	461	15.6	45	9.8	1.5	10	2.2	0.3
Sidechain-Sidechain	172	5.8	17	9.9	0.6	10	5.8	0.3
Sequential ($i-j =1$)	695	23.5	43	6.2	1.5	7	1.0	0.2
Backbone-Backbone	218	7.4	2	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	398	13.4	31	7.8	1.0	5	1.3	0.2
Sidechain-Sidechain	79	2.7	10	12.7	0.3	2	2.5	0.1
Medium range ($i-j >1$ & $i-j <5$)	562	19.0	72	12.8	2.4	19	3.4	0.6
Backbone-Backbone	160	5.4	7	4.4	0.2	4	2.5	0.1
Backbone-Sidechain	273	9.2	30	11.0	1.0	10	3.7	0.3
Sidechain-Sidechain	129	4.4	35	27.1	1.2	5	3.9	0.2
Long range ($i-j \geq 5$)	980	33.1	148	15.1	5.0	14	1.4	0.5
Backbone-Backbone	128	4.3	11	8.6	0.4	1	0.8	0.0
Backbone-Sidechain	451	15.2	46	10.2	1.6	0	0.0	0.0
Sidechain-Sidechain	401	13.5	91	22.7	3.1	13	3.2	0.4
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	2962	100.0	325	11.0	11.0	60	2.0	2.0
Backbone-Backbone	598	20.2	20	3.3	0.7	5	0.8	0.2
Backbone-Sidechain	1583	53.4	152	9.6	5.1	25	1.6	0.8
Sidechain-Sidechain	781	26.4	153	19.6	5.2	30	3.8	1.0

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

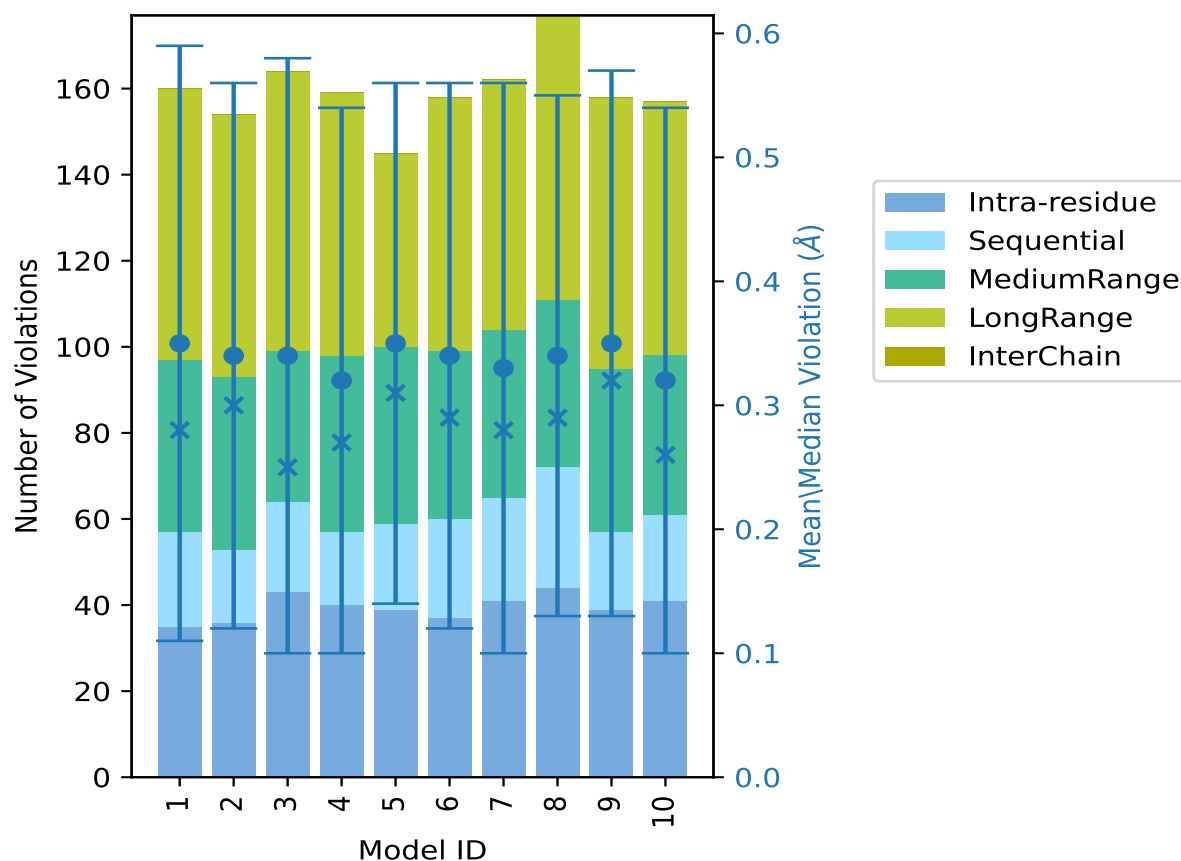
9.2 Distance violation statistics for each model [i](#)

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	35	22	40	63	0	160	0.35	1.47	0.24	0.28
2	36	17	40	61	0	154	0.34	1.27	0.22	0.3
3	43	21	35	65	0	164	0.34	1.21	0.24	0.25
4	40	17	41	61	0	159	0.32	1.51	0.22	0.27
5	39	20	41	45	0	145	0.35	1.04	0.21	0.31
6	37	23	39	59	0	158	0.34	1.23	0.22	0.29
7	41	24	39	58	0	162	0.33	1.54	0.23	0.28
8	44	28	39	66	0	177	0.34	1.01	0.21	0.29
9	39	18	38	63	0	158	0.35	1.49	0.22	0.32
10	41	20	37	59	0	157	0.32	1.52	0.22	0.26

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 [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2637(IR:663, SQ:652, MR:490, LR:832, 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	%
9	8	14	44	0	75	1	10.0
3	5	10	25	0	43	2	20.0
4	5	8	12	0	29	3	30.0

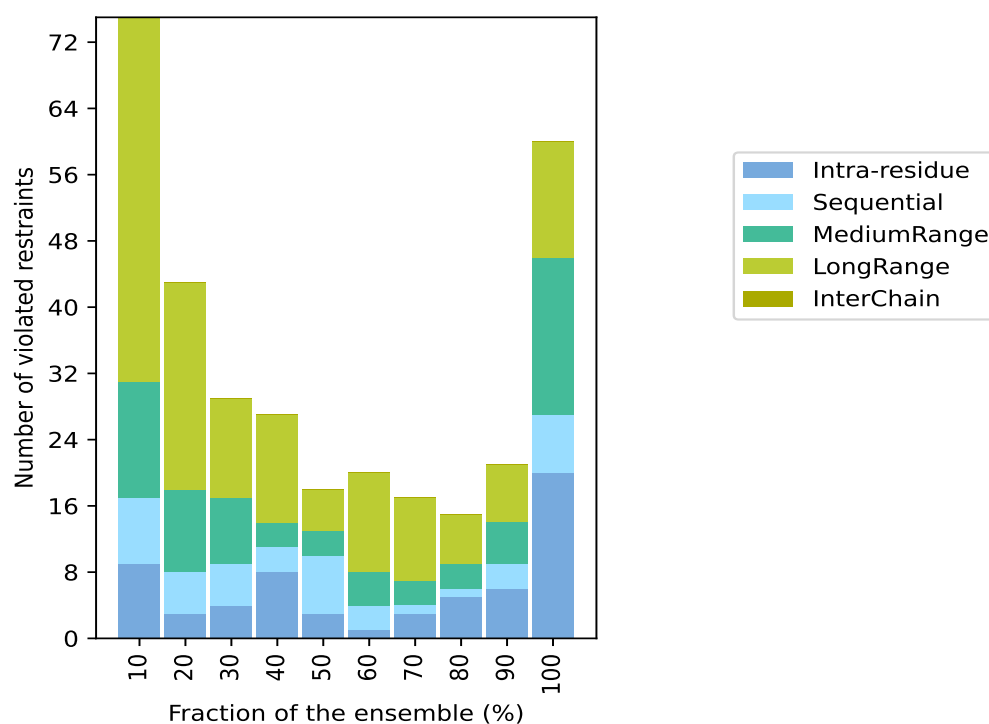
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
8	3	3	13	0	27	4	40.0
3	7	3	5	0	18	5	50.0
1	3	4	12	0	20	6	60.0
3	1	3	10	0	17	7	70.0
5	1	3	6	0	15	8	80.0
6	3	5	7	0	21	9	90.0
20	7	19	14	0	60	10	100.0

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 ⓘ

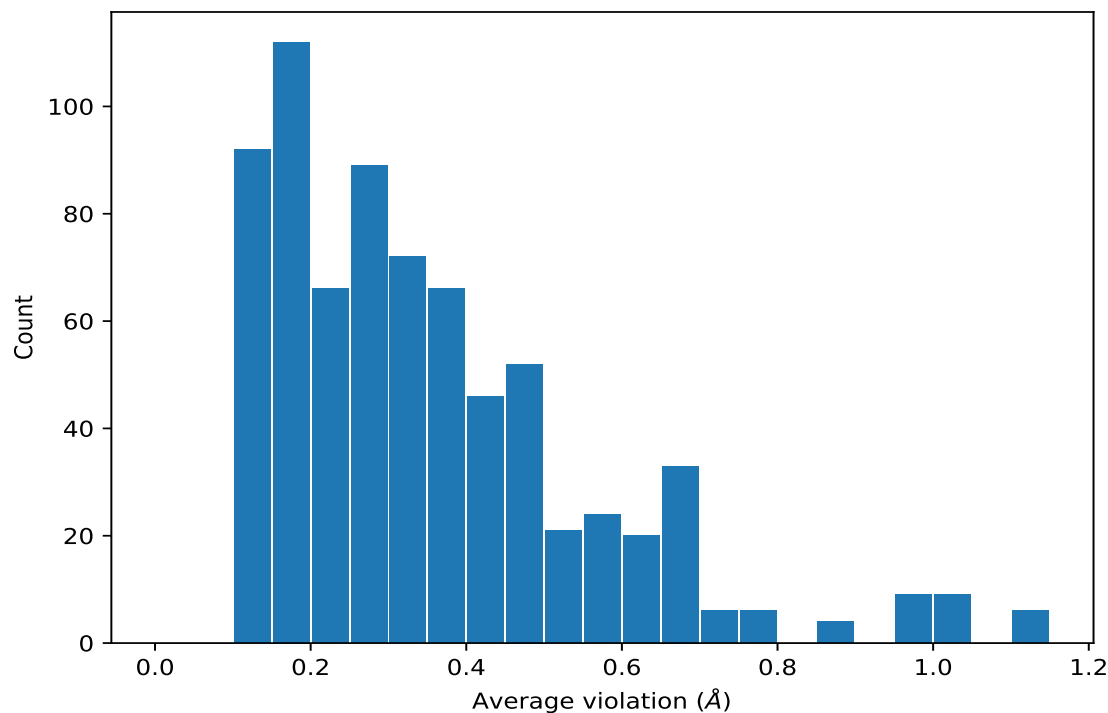


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	10	1.1	0.17	1.19
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	10	1.1	0.17	1.19
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	10	1.1	0.17	1.19
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	10	1.1	0.17	1.19
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	10	1.1	0.17	1.19
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	10	1.1	0.17	1.19
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	10	0.88	0.17	0.89
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	10	0.88	0.17	0.89
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	10	0.88	0.17	0.89
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	10	0.88	0.17	0.89
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	10	0.76	0.09	0.79
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	10	0.76	0.09	0.79
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	10	0.76	0.09	0.79
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	10	0.74	0.11	0.74
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	10	0.74	0.11	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	10	0.74	0.11	0.74
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	10	0.69	0.09	0.65
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	10	0.69	0.09	0.65
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	10	0.69	0.09	0.65
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	10	0.69	0.09	0.65
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	10	0.69	0.09	0.65
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	10	0.69	0.09	0.65
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	10	0.68	0.14	0.72
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	10	0.68	0.14	0.72
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	10	0.68	0.14	0.72
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	10	0.68	0.14	0.72
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	10	0.68	0.14	0.72
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	10	0.68	0.14	0.72
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	10	0.68	0.15	0.68
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	10	0.68	0.15	0.68
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	10	0.68	0.15	0.68
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	10	0.65	0.2	0.76
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	10	0.65	0.2	0.76
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	10	0.65	0.2	0.76
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	10	0.63	0.01	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	10	0.63	0.01	0.64
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	10	0.62	0.02	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	10	0.62	0.02	0.61
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	10	0.61	0.12	0.69
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	10	0.61	0.12	0.69
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	10	0.61	0.12	0.69
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	10	0.61	0.12	0.69
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	10	0.61	0.12	0.69
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	10	0.61	0.12	0.69
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	10	0.61	0.06	0.63
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	10	0.61	0.06	0.63
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	10	0.61	0.06	0.63
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	10	0.6	0.08	0.6
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	10	0.6	0.08	0.6
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	10	0.6	0.08	0.6
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	10	0.59	0.02	0.58
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	10	0.59	0.02	0.58
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	10	0.58	0.15	0.51
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	10	0.58	0.15	0.51
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	10	0.58	0.15	0.51
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	10	0.58	0.01	0.58
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	10	0.58	0.01	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	10	0.56	0.02	0.56
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	10	0.56	0.02	0.56
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	10	0.56	0.02	0.56
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	10	0.56	0.01	0.56
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	10	0.56	0.01	0.56
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	10	0.54	0.14	0.58
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	10	0.54	0.14	0.58
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	10	0.54	0.14	0.58
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	10	0.54	0.14	0.58
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	10	0.54	0.14	0.58
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	10	0.54	0.14	0.58
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	10	0.51	0.06	0.55
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	10	0.51	0.06	0.55
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	10	0.51	0.06	0.55
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	10	0.49	0.03	0.5
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	10	0.49	0.03	0.5
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	10	0.49	0.03	0.5
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	10	0.45	0.03	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	10	0.45	0.03	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	10	0.45	0.03	0.45
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	10	0.44	0.01	0.44
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	10	0.44	0.01	0.44
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	10	0.44	0.01	0.44
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	10	0.44	0.18	0.39
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	10	0.44	0.18	0.39
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	10	0.44	0.18	0.39
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	10	0.43	0.04	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	10	0.43	0.04	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	10	0.43	0.04	0.42
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	10	0.42	0.03	0.4
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	10	0.42	0.03	0.4
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	10	0.41	0.07	0.42
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	10	0.41	0.07	0.42
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	10	0.41	0.07	0.42
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	10	0.39	0.01	0.4
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	10	0.39	0.01	0.4
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	10	0.39	0.01	0.4
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	10	0.39	0.05	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	10	0.39	0.05	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	10	0.39	0.05	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	10	0.39	0.05	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	10	0.39	0.05	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	10	0.39	0.05	0.39
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	10	0.39	0.03	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	10	0.39	0.03	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	10	0.39	0.03	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.39	0.06	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.39	0.06	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.39	0.06	0.4
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	10	0.37	0.07	0.4
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	10	0.37	0.07	0.4
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	10	0.37	0.07	0.4
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	10	0.37	0.05	0.38
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	10	0.37	0.05	0.38
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	10	0.37	0.05	0.38
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	10	0.36	0.07	0.37
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	10	0.36	0.07	0.37
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	10	0.36	0.07	0.37
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	10	0.36	0.08	0.34
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	10	0.36	0.08	0.34
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	10	0.35	0.11	0.3
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	10	0.35	0.11	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	10	0.33	0.07	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	10	0.33	0.07	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	10	0.33	0.07	0.32
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	10	0.3	0.08	0.3
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	10	0.3	0.08	0.3
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	10	0.3	0.08	0.3
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	10	0.29	0.02	0.29
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	10	0.29	0.02	0.29
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	10	0.28	0.04	0.29
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	10	0.28	0.04	0.29
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	10	0.28	0.04	0.29
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	10	0.28	0.04	0.29
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	10	0.28	0.04	0.29
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	10	0.28	0.04	0.29
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	10	0.27	0.08	0.28
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	10	0.27	0.08	0.28
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	10	0.26	0.02	0.26
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	10	0.26	0.02	0.26
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	10	0.26	0.02	0.26
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	10	0.26	0.02	0.26
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	10	0.26	0.02	0.26
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	10	0.26	0.02	0.26
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	10	0.21	0.03	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	10	0.21	0.03	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	10	0.21	0.03	0.2
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	10	0.2	0.02	0.2
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	10	0.2	0.02	0.2
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	10	0.2	0.02	0.2
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	10	0.2	0.05	0.18
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	10	0.2	0.05	0.18
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	10	0.2	0.05	0.18
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	10	0.2	0.06	0.2
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	10	0.2	0.06	0.2
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	10	0.2	0.06	0.2
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	10	0.19	0.02	0.19
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	10	0.18	0.05	0.18
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	10	0.18	0.05	0.18
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	10	0.18	0.05	0.18
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	10	0.18	0.05	0.18
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	10	0.18	0.05	0.18
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	10	0.18	0.05	0.18
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	10	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	10	0.18	0.05	0.18
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	10	0.18	0.05	0.18
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	10	0.15	0.04	0.14
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	10	0.15	0.05	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	10	0.15	0.05	0.13
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	10	0.15	0.02	0.16
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	10	0.15	0.0	0.15
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	10	0.14	0.02	0.14
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	10	0.14	0.01	0.14
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	10	0.13	0.02	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	10	0.13	0.0	0.13
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	10	0.12	0.0	0.12
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	10	0.12	0.0	0.12
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	10	0.12	0.0	0.12
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	9	0.68	0.15	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	9	0.68	0.15	0.76
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	9	0.6	0.22	0.64
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	9	0.6	0.22	0.64
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	9	0.6	0.22	0.64
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	9	0.6	0.22	0.64
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	9	0.43	0.03	0.45
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	9	0.43	0.03	0.45
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	9	0.43	0.03	0.45
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	9	0.42	0.14	0.49
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	9	0.42	0.14	0.49
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	9	0.41	0.03	0.42
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	9	0.41	0.03	0.42
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	9	0.41	0.03	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	9	0.4	0.06	0.42
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	9	0.4	0.06	0.42
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	9	0.4	0.06	0.42
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	9	0.39	0.01	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	9	0.39	0.01	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	9	0.39	0.01	0.4
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	9	0.39	0.1	0.44
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	9	0.39	0.1	0.44
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	9	0.39	0.1	0.44
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	9	0.38	0.11	0.45
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	9	0.38	0.11	0.45
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	9	0.38	0.11	0.45
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	9	0.31	0.15	0.23
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	9	0.31	0.15	0.23
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	9	0.31	0.15	0.23
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	9	0.31	0.12	0.32
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	9	0.31	0.12	0.32
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	9	0.26	0.11	0.27
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	9	0.26	0.11	0.27
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	9	0.25	0.06	0.28
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	9	0.25	0.06	0.28
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	9	0.24	0.08	0.22
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	9	0.24	0.08	0.22
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	9	0.24	0.08	0.22
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	9	0.18	0.06	0.17
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	9	0.18	0.06	0.17
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	9	0.18	0.06	0.16
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	9	0.18	0.06	0.16
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	9	0.18	0.06	0.16
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	9	0.15	0.01	0.15
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	9	0.14	0.02	0.13
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	9	0.13	0.02	0.12
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	9	0.11	0.01	0.11
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	9	0.11	0.01	0.11
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	8	0.69	0.19	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	8	0.69	0.19	0.8
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	8	0.69	0.19	0.8
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	8	0.55	0.06	0.55
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	8	0.55	0.06	0.55
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	8	0.55	0.06	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	8	0.5	0.1	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	8	0.5	0.1	0.55
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	8	0.44	0.02	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	8	0.44	0.02	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	8	0.44	0.02	0.44
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	8	0.41	0.01	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	8	0.41	0.01	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	8	0.41	0.01	0.41
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	8	0.31	0.12	0.28
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	8	0.31	0.12	0.28
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	8	0.31	0.12	0.28
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	8	0.3	0.15	0.34
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	8	0.3	0.15	0.34
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	8	0.29	0.09	0.29
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	8	0.29	0.09	0.29
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	8	0.29	0.09	0.29
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	8	0.26	0.08	0.24
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	8	0.26	0.08	0.24
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	8	0.26	0.08	0.24
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	8	0.26	0.08	0.24
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	8	0.26	0.08	0.24
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	8	0.26	0.08	0.24
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	8	0.24	0.11	0.24
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	8	0.24	0.11	0.24
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	8	0.24	0.11	0.24
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	8	0.21	0.04	0.22
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	8	0.21	0.04	0.22
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	8	0.18	0.08	0.15
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	8	0.18	0.08	0.15
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	8	0.18	0.08	0.14
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	8	0.18	0.08	0.14
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	8	0.18	0.08	0.14
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	8	0.18	0.05	0.2
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	8	0.18	0.05	0.2
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	8	0.18	0.05	0.2
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	8	0.12	0.01	0.12
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	7	1.0	0.37	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	7	1.0	0.37	0.94
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	7	1.0	0.37	0.94
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	7	1.0	0.37	0.94
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	7	1.0	0.37	0.94
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	7	1.0	0.37	0.94
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	7	1.0	0.37	0.94
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	7	1.0	0.37	0.94
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	7	1.0	0.37	0.94
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	7	0.97	0.61	1.44
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	7	0.97	0.61	1.44
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	7	0.79	0.26	0.89
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	7	0.79	0.26	0.89
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	7	0.79	0.26	0.89
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	7	0.58	0.01	0.58
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	7	0.58	0.01	0.58
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	7	0.45	0.26	0.4
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	7	0.45	0.26	0.4
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	7	0.45	0.26	0.4
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	7	0.38	0.16	0.41
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	7	0.38	0.16	0.41
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	7	0.35	0.02	0.35
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	7	0.35	0.02	0.35
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	7	0.35	0.1	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	7	0.35	0.1	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	7	0.35	0.1	0.42
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	7	0.3	0.01	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	7	0.3	0.01	0.3
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	7	0.3	0.15	0.25
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	7	0.3	0.15	0.25
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	7	0.3	0.15	0.25
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	7	0.3	0.15	0.25
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	7	0.29	0.11	0.25
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	7	0.29	0.11	0.25
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	7	0.29	0.11	0.25
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	7	0.23	0.05	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	7	0.23	0.05	0.24
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	7	0.23	0.05	0.24
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	7	0.18	0.06	0.16
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	7	0.18	0.06	0.16
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	7	0.16	0.04	0.16
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	7	0.14	0.01	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	7	0.14	0.01	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	7	0.14	0.01	0.14
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	7	0.13	0.02	0.13
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE1	6	0.74	0.15	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE2	6	0.74	0.15	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE3	6	0.74	0.15	0.84
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG21	6	0.53	0.01	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG22	6	0.53	0.01	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG23	6	0.53	0.01	0.52
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE2	6	0.45	0.17	0.56
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE3	6	0.45	0.17	0.56
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG21	6	0.38	0.01	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG22	6	0.38	0.01	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG23	6	0.38	0.01	0.38
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE1	6	0.38	0.26	0.22
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE2	6	0.38	0.26	0.22
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE3	6	0.38	0.26	0.22
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD11	6	0.34	0.09	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD12	6	0.34	0.09	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD13	6	0.34	0.09	0.4
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG21	6	0.31	0.09	0.28
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG22	6	0.31	0.09	0.28
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG23	6	0.31	0.09	0.28
(1,2197)	1:88:A:LEU:HD11	1:89:A:GLY:H	6	0.31	0.13	0.34
(1,2197)	1:88:A:LEU:HD12	1:89:A:GLY:H	6	0.31	0.13	0.34
(1,2197)	1:88:A:LEU:HD13	1:89:A:GLY:H	6	0.31	0.13	0.34
(1,2197)	1:88:A:LEU:HD21	1:89:A:GLY:H	6	0.31	0.13	0.34
(1,2197)	1:88:A:LEU:HD22	1:89:A:GLY:H	6	0.31	0.13	0.34
(1,2197)	1:88:A:LEU:HD23	1:89:A:GLY:H	6	0.31	0.13	0.34
(1,2172)	1:87:A:LEU:HD11	1:91:A:ASN:HB2	6	0.29	0.07	0.27
(1,2172)	1:87:A:LEU:HD12	1:91:A:ASN:HB2	6	0.29	0.07	0.27
(1,2172)	1:87:A:LEU:HD13	1:91:A:ASN:HB2	6	0.29	0.07	0.27
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG11	6	0.29	0.13	0.29
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG12	6	0.29	0.13	0.29
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG13	6	0.29	0.13	0.29
(1,1336)	1:46:A:THR:HG21	1:47:A:TYR:H	6	0.25	0.1	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1336)	1:46:A:THR:HG22	1:47:A:TYR:H	6	0.25	0.1	0.2
(1,1336)	1:46:A:THR:HG23	1:47:A:TYR:H	6	0.25	0.1	0.2
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB1	6	0.25	0.09	0.24
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB2	6	0.25	0.09	0.24
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB3	6	0.25	0.09	0.24
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE1	6	0.24	0.09	0.23
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE2	6	0.24	0.09	0.23
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG11	6	0.23	0.05	0.23
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG12	6	0.23	0.05	0.23
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG13	6	0.23	0.05	0.23
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG11	6	0.23	0.05	0.23
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG12	6	0.23	0.05	0.23
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG13	6	0.23	0.05	0.23
(1,431)	1:15:A:ILE:HG21	1:81:A:GLY:HA2	6	0.23	0.08	0.21
(1,431)	1:15:A:ILE:HG22	1:81:A:GLY:HA2	6	0.23	0.08	0.21
(1,431)	1:15:A:ILE:HG23	1:81:A:GLY:HA2	6	0.23	0.08	0.21
(1,2542)	1:26:A:PHE:HE1	1:55:A:VAL:HA	6	0.18	0.07	0.16
(1,2542)	1:26:A:PHE:HE2	1:55:A:VAL:HA	6	0.18	0.07	0.16
(1,2407)	1:99:A:ILE:HA	1:104:A:ALA:H	6	0.15	0.01	0.15
(1,2468)	1:101:A:LYS:HB2	1:103:A:ALA:H	6	0.14	0.04	0.12
(1,401)	1:15:A:ILE:HG13	1:21:A:VAL:HB	6	0.12	0.01	0.12
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB1	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB2	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB3	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB1	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB2	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB3	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB1	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB2	6	0.1	0.0	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB3	6	0.1	0.0	0.11
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE1	5	0.49	0.26	0.7
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE2	5	0.49	0.26	0.7
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE1	5	0.49	0.26	0.7
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE2	5	0.49	0.26	0.7
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE1	5	0.49	0.26	0.7
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE2	5	0.49	0.26	0.7
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE2	5	0.45	0.14	0.55
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE3	5	0.45	0.14	0.55
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE1	5	0.31	0.06	0.33
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE2	5	0.31	0.06	0.33
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD11	5	0.28	0.08	0.28
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD12	5	0.28	0.08	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD13	5	0.28	0.08	0.28
(1,2200)	1:88:A:LEU:HD21	1:88:A:LEU:HA	5	0.23	0.09	0.21
(1,2200)	1:88:A:LEU:HD22	1:88:A:LEU:HA	5	0.23	0.09	0.21
(1,2200)	1:88:A:LEU:HD23	1:88:A:LEU:HA	5	0.23	0.09	0.21
(1,1225)	1:41:A:GLU:HG2	1:42:A:GLU:H	5	0.2	0.04	0.19
(1,1225)	1:41:A:GLU:HG3	1:42:A:GLU:H	5	0.2	0.04	0.19
(1,1331)	1:46:A:THR:HG21	1:47:A:TYR:HA	5	0.18	0.01	0.17
(1,1331)	1:46:A:THR:HG22	1:47:A:TYR:HA	5	0.18	0.01	0.17
(1,1331)	1:46:A:THR:HG23	1:47:A:TYR:HA	5	0.18	0.01	0.17
(1,1550)	1:57:A:VAL:HG21	1:58:A:ASP:H	5	0.18	0.05	0.17
(1,1550)	1:57:A:VAL:HG22	1:58:A:ASP:H	5	0.18	0.05	0.17
(1,1550)	1:57:A:VAL:HG23	1:58:A:ASP:H	5	0.18	0.05	0.17
(1,380)	1:15:A:ILE:HD11	1:23:A:VAL:HB	5	0.17	0.03	0.15
(1,380)	1:15:A:ILE:HD12	1:23:A:VAL:HB	5	0.17	0.03	0.15
(1,380)	1:15:A:ILE:HD13	1:23:A:VAL:HB	5	0.17	0.03	0.15
(1,1737)	1:69:A:ILE:HD11	1:69:A:ILE:HA	5	0.16	0.03	0.16
(1,1737)	1:69:A:ILE:HD12	1:69:A:ILE:HA	5	0.16	0.03	0.16
(1,1737)	1:69:A:ILE:HD13	1:69:A:ILE:HA	5	0.16	0.03	0.16
(1,2535)	1:103:A:ALA:H	1:104:A:ALA:HA	5	0.15	0.02	0.15
(1,1505)	1:54:A:LYS:HA	1:54:A:LYS:HG3	5	0.14	0.03	0.13
(1,780)	1:24:A:ASP:HB3	1:26:A:PHE:H	5	0.13	0.01	0.13
(1,1703)	1:67:A:GLU:H	1:68:A:ASN:HB2	5	0.13	0.01	0.13
(1,1988)	1:77:A:VAL:H	1:84:A:VAL:HB	5	0.13	0.02	0.12
(1,2506)	1:101:A:LYS:H	1:103:A:ALA:H	5	0.13	0.01	0.13
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG11	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG12	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG13	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG11	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG12	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG13	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG11	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG12	5	0.13	0.03	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG13	5	0.13	0.03	0.1
(2,166)	1:28:A:GLU:H	1:29:A:TRP:HE1	5	0.11	0.0	0.11
(2,10)	1:1:A:SER:HB2	1:3:A:LYS:H	4	0.59	0.05	0.62
(2,10)	1:1:A:SER:HB3	1:3:A:LYS:H	4	0.59	0.05	0.62
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG11	4	0.57	0.01	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG12	4	0.57	0.01	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG13	4	0.57	0.01	0.57
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE2	4	0.55	0.02	0.56
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE3	4	0.55	0.02	0.56
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE1	4	0.52	0.2	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE2	4	0.52	0.2	0.53
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE3	4	0.52	0.2	0.53
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD1	4	0.47	0.14	0.51
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD2	4	0.47	0.14	0.51
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD1	4	0.47	0.14	0.51
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD2	4	0.47	0.14	0.51
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD1	4	0.47	0.14	0.51
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD2	4	0.47	0.14	0.51
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG21	4	0.41	0.05	0.43
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG22	4	0.41	0.05	0.43
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG23	4	0.41	0.05	0.43
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG11	4	0.37	0.04	0.38
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG12	4	0.37	0.04	0.38
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG13	4	0.37	0.04	0.38
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB1	4	0.34	0.09	0.3
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB2	4	0.34	0.09	0.3
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB3	4	0.34	0.09	0.3
(1,1959)	1:77:A:VAL:HG11	1:102:A:TYR:HB2	4	0.31	0.11	0.3
(1,1959)	1:77:A:VAL:HG12	1:102:A:TYR:HB2	4	0.31	0.11	0.3
(1,1959)	1:77:A:VAL:HG13	1:102:A:TYR:HB2	4	0.31	0.11	0.3
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE1	4	0.3	0.12	0.3
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE2	4	0.3	0.12	0.3
(1,1376)	1:47:A:TYR:HD1	1:99:A:ILE:HG12	4	0.29	0.02	0.29
(1,1376)	1:47:A:TYR:HD2	1:99:A:ILE:HG12	4	0.29	0.02	0.29
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD21	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD22	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD23	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD21	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD22	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD23	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD21	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD22	4	0.27	0.04	0.28
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD23	4	0.27	0.04	0.28
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD1	4	0.26	0.06	0.26
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD2	4	0.26	0.06	0.26
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD1	4	0.26	0.06	0.26
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD2	4	0.26	0.06	0.26
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD1	4	0.26	0.06	0.26
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD2	4	0.26	0.06	0.26
(1,826)	1:25:A:PHE:HD1	1:25:A:PHE:H	4	0.25	0.0	0.25
(1,826)	1:25:A:PHE:HD2	1:25:A:PHE:H	4	0.25	0.0	0.25
(1,112)	1:6:A:THR:H	1:6:A:THR:HG21	4	0.24	0.03	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,112)	1:6:A:THR:H	1:6:A:THR:HG22	4	0.24	0.03	0.25
(1,112)	1:6:A:THR:H	1:6:A:THR:HG23	4	0.24	0.03	0.25
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG2	4	0.19	0.05	0.18
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG3	4	0.19	0.05	0.18
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD11	4	0.19	0.02	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD12	4	0.19	0.02	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD13	4	0.19	0.02	0.2
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG21	4	0.18	0.03	0.18
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG22	4	0.18	0.03	0.18
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG23	4	0.18	0.03	0.18
(1,1079)	1:36:A:ILE:HG21	1:37:A:ALA:H	4	0.17	0.03	0.18
(1,1079)	1:36:A:ILE:HG22	1:37:A:ALA:H	4	0.17	0.03	0.18
(1,1079)	1:36:A:ILE:HG23	1:37:A:ALA:H	4	0.17	0.03	0.18
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB1	4	0.16	0.04	0.14
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB2	4	0.16	0.04	0.14
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB3	4	0.16	0.04	0.14
(1,433)	1:15:A:ILE:HG21	1:82:A:SER:HA	4	0.12	0.01	0.12
(1,433)	1:15:A:ILE:HG22	1:82:A:SER:HA	4	0.12	0.01	0.12
(1,433)	1:15:A:ILE:HG23	1:82:A:SER:HA	4	0.12	0.01	0.12
(1,1218)	1:40:A:TYR:H	1:92:A:ASP:HA	4	0.12	0.02	0.12
(1,1739)	1:69:A:ILE:HD11	1:69:A:ILE:HG13	4	0.12	0.01	0.12
(1,1739)	1:69:A:ILE:HD12	1:69:A:ILE:HG13	4	0.12	0.01	0.12
(1,1739)	1:69:A:ILE:HD13	1:69:A:ILE:HG13	4	0.12	0.01	0.12
(1,43)	1:3:A:LYS:HG3	1:4:A:ILE:H	4	0.12	0.01	0.12
(1,460)	1:17:A:GLN:HA	1:17:A:GLN:HG2	4	0.12	0.01	0.12
(1,1740)	1:69:A:ILE:HD11	1:69:A:ILE:HG12	4	0.12	0.01	0.12
(1,1740)	1:69:A:ILE:HD12	1:69:A:ILE:HG12	4	0.12	0.01	0.12
(1,1740)	1:69:A:ILE:HD13	1:69:A:ILE:HG12	4	0.12	0.01	0.12
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB1	4	0.11	0.01	0.11
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB2	4	0.11	0.01	0.11
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB3	4	0.11	0.01	0.11
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD11	3	0.48	0.2	0.47
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD12	3	0.48	0.2	0.47
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD13	3	0.48	0.2	0.47
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD11	3	0.43	0.3	0.34
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD12	3	0.43	0.3	0.34
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD13	3	0.43	0.3	0.34
(1,747)	1:23:A:VAL:HG21	1:53:A:ILE:HG12	3	0.42	0.06	0.46
(1,747)	1:23:A:VAL:HG22	1:53:A:ILE:HG12	3	0.42	0.06	0.46
(1,747)	1:23:A:VAL:HG23	1:53:A:ILE:HG12	3	0.42	0.06	0.46
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE1	3	0.42	0.21	0.37
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE2	3	0.42	0.21	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE1	3	0.42	0.21	0.37
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE2	3	0.42	0.21	0.37
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE1	3	0.42	0.21	0.37
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE2	3	0.42	0.21	0.37
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB2	3	0.37	0.01	0.38
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	3	0.37	0.01	0.38
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD1	3	0.36	0.0	0.36
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD2	3	0.36	0.0	0.36
(1,2388)	1:98:A:LEU:HD21	1:99:A:ILE:HA	3	0.32	0.11	0.25
(1,2388)	1:98:A:LEU:HD22	1:99:A:ILE:HA	3	0.32	0.11	0.25
(1,2388)	1:98:A:LEU:HD23	1:99:A:ILE:HA	3	0.32	0.11	0.25
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG21	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG22	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG23	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG21	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG22	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG23	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG21	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG22	3	0.31	0.03	0.32
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG23	3	0.31	0.03	0.32
(1,2549)	1:27:A:ALA:HB1	1:30:A:CYS:HB3	3	0.26	0.1	0.31
(1,2549)	1:27:A:ALA:HB2	1:30:A:CYS:HB3	3	0.26	0.1	0.31
(1,2549)	1:27:A:ALA:HB3	1:30:A:CYS:HB3	3	0.26	0.1	0.31
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD1	3	0.25	0.05	0.26
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD2	3	0.25	0.05	0.26
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB1	3	0.23	0.11	0.17
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB2	3	0.23	0.11	0.17
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB3	3	0.23	0.11	0.17
(1,96)	1:5:A:VAL:H	1:5:A:VAL:HB	3	0.21	0.01	0.21
(1,668)	1:22:A:ILE:HG21	1:52:A:PHE:HA	3	0.2	0.04	0.23
(1,668)	1:22:A:ILE:HG22	1:52:A:PHE:HA	3	0.2	0.04	0.23
(1,668)	1:22:A:ILE:HG23	1:52:A:PHE:HA	3	0.2	0.04	0.23
(1,1488)	1:52:A:PHE:HZ	1:99:A:ILE:HG12	3	0.19	0.05	0.17
(1,153)	1:8:A:GLN:HE22	1:9:A:SER:H	3	0.16	0.0	0.16
(1,654)	1:22:A:ILE:HD11	1:75:A:PHE:HB3	3	0.16	0.06	0.14
(1,654)	1:22:A:ILE:HD12	1:75:A:PHE:HB3	3	0.16	0.06	0.14
(1,654)	1:22:A:ILE:HD13	1:75:A:PHE:HB3	3	0.16	0.06	0.14
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB1	3	0.16	0.04	0.15
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB2	3	0.16	0.04	0.15
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB3	3	0.16	0.04	0.15
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB1	3	0.16	0.04	0.15
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB2	3	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB3	3	0.16	0.04	0.15
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB1	3	0.16	0.04	0.15
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB2	3	0.16	0.04	0.15
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB3	3	0.16	0.04	0.15
(2,243)	1:47:A:TYR:HA	1:50:A:MET:HB2	3	0.16	0.02	0.17
(1,2415)	1:99:A:ILE:HD11	1:103:A:ALA:H	3	0.15	0.04	0.13
(1,2415)	1:99:A:ILE:HD12	1:103:A:ALA:H	3	0.15	0.04	0.13
(1,2415)	1:99:A:ILE:HD13	1:103:A:ALA:H	3	0.15	0.04	0.13
(1,105)	1:5:A:VAL:H	1:55:A:VAL:HB	3	0.14	0.04	0.12
(1,44)	1:3:A:LYS:HG3	1:53:A:ILE:HA	3	0.12	0.01	0.12
(1,1133)	1:39:A:PHE:HB2	1:41:A:GLU:H	3	0.12	0.01	0.12
(1,2463)	1:101:A:LYS:HA	1:104:A:ALA:H	3	0.12	0.01	0.11
(2,19)	1:2:A:VAL:HB	1:3:A:LYS:HA	3	0.12	0.02	0.11
(1,586)	1:20:A:LEU:HG	1:51:A:VAL:H	3	0.12	0.02	0.11
(1,1486)	1:52:A:PHE:HZ	1:99:A:ILE:HA	3	0.12	0.02	0.11
(1,54)	1:3:A:LYS:H	1:3:A:LYS:HG2	3	0.12	0.0	0.12
(1,164)	1:8:A:GLN:H	1:8:A:GLN:HG2	3	0.11	0.01	0.12
(2,197)	1:36:A:ILE:HA	1:92:A:ASP:H	3	0.11	0.01	0.1
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE1	2	0.68	0.21	0.68
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE2	2	0.68	0.21	0.68
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE3	2	0.68	0.21	0.68
(1,2475)	1:101:A:LYS:HE2	1:102:A:TYR:HE1	2	0.5	0.05	0.5
(1,2475)	1:101:A:LYS:HE2	1:102:A:TYR:HE2	2	0.5	0.05	0.5
(1,2475)	1:101:A:LYS:HE3	1:102:A:TYR:HE1	2	0.5	0.05	0.5
(1,2475)	1:101:A:LYS:HE3	1:102:A:TYR:HE2	2	0.5	0.05	0.5
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG21	2	0.49	0.33	0.49
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG22	2	0.49	0.33	0.49
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG23	2	0.49	0.33	0.49
(1,1631)	1:63:A:VAL:HG11	1:66:A:LYS:HG2	2	0.48	0.02	0.48
(1,1631)	1:63:A:VAL:HG11	1:66:A:LYS:HG3	2	0.48	0.02	0.48
(1,1631)	1:63:A:VAL:HG12	1:66:A:LYS:HG2	2	0.48	0.02	0.48
(1,1631)	1:63:A:VAL:HG12	1:66:A:LYS:HG3	2	0.48	0.02	0.48
(1,1631)	1:63:A:VAL:HG13	1:66:A:LYS:HG2	2	0.48	0.02	0.48
(1,1631)	1:63:A:VAL:HG13	1:66:A:LYS:HG3	2	0.48	0.02	0.48
(2,209)	1:40:A:TYR:HD1	1:43:A:CYS:H	2	0.38	0.05	0.38
(2,209)	1:40:A:TYR:HD2	1:43:A:CYS:H	2	0.38	0.05	0.38
(1,1960)	1:77:A:VAL:HG11	1:102:A:TYR:HD1	2	0.33	0.04	0.33
(1,1960)	1:77:A:VAL:HG11	1:102:A:TYR:HD2	2	0.33	0.04	0.33
(1,1960)	1:77:A:VAL:HG12	1:102:A:TYR:HD1	2	0.33	0.04	0.33
(1,1960)	1:77:A:VAL:HG12	1:102:A:TYR:HD2	2	0.33	0.04	0.33
(1,1960)	1:77:A:VAL:HG13	1:102:A:TYR:HD1	2	0.33	0.04	0.33
(1,1960)	1:77:A:VAL:HG13	1:102:A:TYR:HD2	2	0.33	0.04	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2271)	1:93:A:SER:HB2	1:97:A:GLN:HE22	2	0.31	0.04	0.31
(1,2271)	1:93:A:SER:HB3	1:97:A:GLN:HE22	2	0.31	0.04	0.31
(1,798)	1:25:A:PHE:HA	1:25:A:PHE:HD1	2	0.3	0.01	0.3
(1,798)	1:25:A:PHE:HA	1:25:A:PHE:HD2	2	0.3	0.01	0.3
(2,34)	1:3:A:LYS:HE2	1:5:A:VAL:HB	2	0.3	0.06	0.3
(2,34)	1:3:A:LYS:HE3	1:5:A:VAL:HB	2	0.3	0.06	0.3
(1,2052)	1:79:A:LYS:HD2	1:80:A:ASN:H	2	0.3	0.0	0.3
(1,2052)	1:79:A:LYS:HD3	1:80:A:ASN:H	2	0.3	0.0	0.3
(2,229)	1:44:A:SER:HG	1:45:A:LYS:HD2	2	0.3	0.18	0.3
(2,229)	1:44:A:SER:HG	1:45:A:LYS:HD3	2	0.3	0.18	0.3
(2,79)	1:12:A:ASP:HB3	1:66:A:LYS:HD2	2	0.29	0.15	0.29
(2,79)	1:12:A:ASP:HB3	1:66:A:LYS:HD3	2	0.29	0.15	0.29
(1,1054)	1:36:A:ILE:HD11	1:91:A:ASN:H	2	0.27	0.03	0.27
(1,1054)	1:36:A:ILE:HD12	1:91:A:ASN:H	2	0.27	0.03	0.27
(1,1054)	1:36:A:ILE:HD13	1:91:A:ASN:H	2	0.27	0.03	0.27
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB1	2	0.26	0.09	0.26
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB2	2	0.26	0.09	0.26
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB3	2	0.26	0.09	0.26
(2,151)	1:27:A:ALA:HB1	1:58:A:ASP:HB2	2	0.25	0.05	0.25
(2,151)	1:27:A:ALA:HB2	1:58:A:ASP:HB2	2	0.25	0.05	0.25
(2,151)	1:27:A:ALA:HB3	1:58:A:ASP:HB2	2	0.25	0.05	0.25
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD11	2	0.24	0.01	0.24
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD12	2	0.24	0.01	0.24
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD13	2	0.24	0.01	0.24
(1,665)	1:22:A:ILE:HG21	1:50:A:MET:HB3	2	0.24	0.02	0.24
(1,665)	1:22:A:ILE:HG22	1:50:A:MET:HB3	2	0.24	0.02	0.24
(1,665)	1:22:A:ILE:HG23	1:50:A:MET:HB3	2	0.24	0.02	0.24
(1,746)	1:23:A:VAL:HG21	1:53:A:ILE:HG13	2	0.22	0.07	0.22
(1,746)	1:23:A:VAL:HG22	1:53:A:ILE:HG13	2	0.22	0.07	0.22
(1,746)	1:23:A:VAL:HG23	1:53:A:ILE:HG13	2	0.22	0.07	0.22
(1,1685)	1:66:A:LYS:HG2	1:67:A:GLU:H	2	0.22	0.07	0.22
(1,1685)	1:66:A:LYS:HG3	1:67:A:GLU:H	2	0.22	0.07	0.22
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG11	2	0.21	0.05	0.21
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG12	2	0.21	0.05	0.21
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG13	2	0.21	0.05	0.21
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB1	2	0.21	0.05	0.21
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB2	2	0.21	0.05	0.21
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB3	2	0.21	0.05	0.21
(1,2550)	1:27:A:ALA:HB1	1:30:A:CYS:HB2	2	0.18	0.02	0.18
(1,2550)	1:27:A:ALA:HB2	1:30:A:CYS:HB2	2	0.18	0.02	0.18
(1,2550)	1:27:A:ALA:HB3	1:30:A:CYS:HB2	2	0.18	0.02	0.18
(1,900)	1:26:A:PHE:HE1	1:54:A:LYS:HB2	2	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,900)	1:26:A:PHE:HE1	1:54:A:LYS:HB3	2	0.18	0.02	0.18
(1,900)	1:26:A:PHE:HE2	1:54:A:LYS:HB2	2	0.18	0.02	0.18
(1,900)	1:26:A:PHE:HE2	1:54:A:LYS:HB3	2	0.18	0.02	0.18
(1,1088)	1:36:A:ILE:HG21	1:75:A:PHE:HZ	2	0.18	0.06	0.18
(1,1088)	1:36:A:ILE:HG22	1:75:A:PHE:HZ	2	0.18	0.06	0.18
(1,1088)	1:36:A:ILE:HG23	1:75:A:PHE:HZ	2	0.18	0.06	0.18
(1,1915)	1:76:A:LYS:HD2	1:86:A:THR:HA	2	0.18	0.02	0.18
(1,1915)	1:76:A:LYS:HD3	1:86:A:THR:HA	2	0.18	0.02	0.18
(2,385)	1:79:A:LYS:HD2	1:81:A:GLY:H	2	0.18	0.03	0.18
(2,385)	1:79:A:LYS:HD3	1:81:A:GLY:H	2	0.18	0.03	0.18
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG21	2	0.17	0.02	0.17
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG22	2	0.17	0.02	0.17
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG23	2	0.17	0.02	0.17
(1,425)	1:15:A:ILE:HG21	1:78:A:TYR:HB2	2	0.17	0.02	0.17
(1,425)	1:15:A:ILE:HG22	1:78:A:TYR:HB2	2	0.17	0.02	0.17
(1,425)	1:15:A:ILE:HG23	1:78:A:TYR:HB2	2	0.17	0.02	0.17
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG21	2	0.16	0.04	0.16
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG22	2	0.16	0.04	0.16
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG23	2	0.16	0.04	0.16
(1,788)	1:24:A:ASP:HB2	1:75:A:PHE:HE1	2	0.15	0.03	0.15
(1,788)	1:24:A:ASP:HB2	1:75:A:PHE:HE2	2	0.15	0.03	0.15
(1,83)	1:5:A:VAL:HG11	1:11:A:PHE:HA	2	0.14	0.03	0.14
(1,83)	1:5:A:VAL:HG12	1:11:A:PHE:HA	2	0.14	0.03	0.14
(1,83)	1:5:A:VAL:HG13	1:11:A:PHE:HA	2	0.14	0.03	0.14
(1,1433)	1:50:A:MET:HG3	1:103:A:ALA:H	2	0.14	0.02	0.14
(1,1607)	1:62:A:GLU:HB3	1:63:A:VAL:H	2	0.14	0.01	0.14
(1,2473)	1:101:A:LYS:HE2	1:101:A:LYS:HG3	2	0.14	0.01	0.14
(1,2473)	1:101:A:LYS:HE3	1:101:A:LYS:HG3	2	0.14	0.01	0.14
(1,753)	1:23:A:VAL:HG21	1:55:A:VAL:H	2	0.12	0.02	0.12
(1,753)	1:23:A:VAL:HG22	1:55:A:VAL:H	2	0.12	0.02	0.12
(1,753)	1:23:A:VAL:HG23	1:55:A:VAL:H	2	0.12	0.02	0.12
(1,1075)	1:36:A:ILE:HG12	1:75:A:PHE:HZ	2	0.12	0.01	0.12
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD21	2	0.12	0.02	0.12
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD22	2	0.12	0.02	0.12
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD23	2	0.12	0.02	0.12
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD21	2	0.12	0.02	0.12
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD22	2	0.12	0.02	0.12
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD23	2	0.12	0.02	0.12
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG21	2	0.12	0.01	0.12
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG22	2	0.12	0.01	0.12
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG23	2	0.12	0.01	0.12
(2,373)	1:77:A:VAL:H	1:83:A:SER:HA	2	0.12	0.01	0.12

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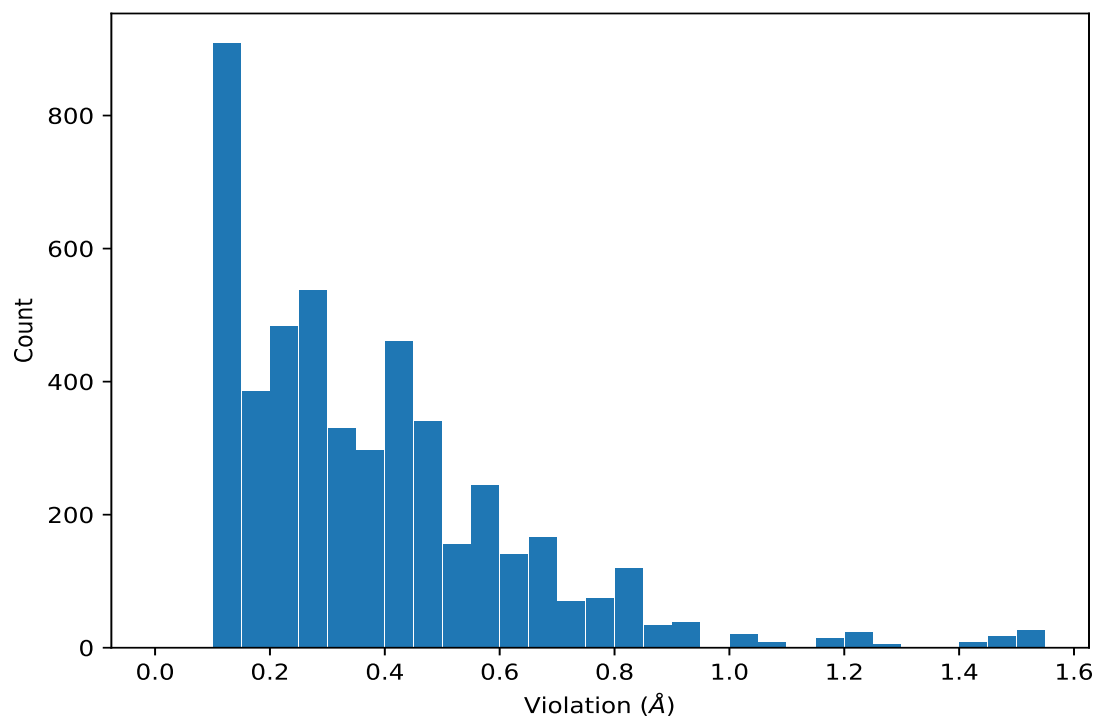
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1259)	1:43:A:CYS:HA	1:52:A:PHE:HZ	2	0.11	0.0	0.11
(1,1432)	1:50:A:MET:HG3	1:52:A:PHE:HZ	2	0.11	0.0	0.11
(2,89)	1:14:A:ILE:H	1:17:A:GLN:HB2	2	0.11	0.01	0.11
(1,47)	1:3:A:LYS:HG2	1:53:A:ILE:HA	2	0.11	0.0	0.11

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)
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	7	1.54
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	7	1.54
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	7	1.54
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	7	1.54
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	7	1.54
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	7	1.54
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	7	1.54
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	7	1.54
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	7	1.54
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	10	1.52
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	10	1.52
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	10	1.52
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	10	1.52
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	10	1.52
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	10	1.52
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	10	1.52
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	10	1.52
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	10	1.52
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	4	1.51
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	4	1.51
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	4	1.51
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	4	1.51
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	4	1.51
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	4	1.51
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	4	1.51
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	4	1.51
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	4	1.51
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	9	1.49
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	9	1.49
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	9	1.49
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	9	1.49
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	9	1.49
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	9	1.49
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	9	1.49
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	9	1.49
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	9	1.49
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	1	1.47
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	1	1.47
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	1	1.47
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	1	1.47
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	1	1.47
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	1	1.47
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	1	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	1	1.47
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	1	1.47
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	1	1.44
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	1	1.44
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	1	1.44
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	1	1.44
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	1	1.44
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	1	1.44
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	1	1.44
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	1	1.44
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	1	1.44
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	2	1.27
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	2	1.27
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	2	1.27
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	2	1.27
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	2	1.27
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	2	1.27
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	4	1.23
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	4	1.23
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	4	1.23
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	4	1.23
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	4	1.23
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	4	1.23
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	6	1.23
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	6	1.23
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	6	1.23
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	6	1.23
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	6	1.23
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	6	1.23
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	10	1.23
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	10	1.23
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	10	1.23
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	10	1.23
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	10	1.23
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	10	1.23
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	3	1.21
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	3	1.21
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	3	1.21
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	3	1.21
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	3	1.21
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	3	1.21
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	3	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	3	1.18
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	3	1.18
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	3	1.18
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	3	1.18
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	3	1.18
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	3	1.18
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	3	1.18
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	3	1.18
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	1	1.17
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	1	1.17
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	1	1.17
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	1	1.17
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	1	1.17
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	1	1.17
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	3	1.09
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	3	1.09
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	3	1.09
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	3	1.09
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	2	1.06
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	2	1.06
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	2	1.06
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	2	1.06
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	5	1.04
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	5	1.04
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	5	1.04
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	5	1.04
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	5	1.04
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	5	1.04
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	5	1.03
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	5	1.03
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	5	1.03
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	5	1.03
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	8	1.01
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	8	1.01
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	8	1.01
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	8	1.01
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	7	1.0
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	7	1.0
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	7	1.0
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	7	1.0
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	7	1.0
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	7	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	6	0.94
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	6	0.94
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	6	0.94
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	6	0.94
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	6	0.94
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	6	0.94
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	6	0.94
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	6	0.94
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	6	0.94
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	3	0.92
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	3	0.92
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	3	0.92
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	8	0.92
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	8	0.92
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	8	0.92
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	8	0.92
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	8	0.92
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	8	0.92
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	6	0.92
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	6	0.92
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	6	0.92
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	6	0.92
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	5	0.91
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	5	0.91
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	5	0.91
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	7	0.91
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	7	0.91
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	7	0.91
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	2	0.9
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	2	0.9
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	2	0.9
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	9	0.9
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	9	0.9
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	9	0.9
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	1	0.9
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	1	0.9
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	1	0.9
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	1	0.9
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	3	0.89
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	3	0.89
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	3	0.89
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	6	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	6	0.89
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	6	0.89
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE1	7	0.89
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE2	7	0.89
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE3	7	0.89
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	8	0.88
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	8	0.88
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	8	0.88
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	9	0.88
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	9	0.88
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	9	0.88
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	9	0.88
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	4	0.88
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	4	0.88
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	4	0.88
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	4	0.88
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	4	0.88
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	4	0.88
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	7	0.87
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	7	0.87
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	7	0.87
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	10	0.86
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	10	0.86
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	10	0.86
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	5	0.86
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	5	0.86
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	5	0.86
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	5	0.86
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	5	0.86
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	5	0.86
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	3	0.85
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	3	0.85
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	3	0.85
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	8	0.85
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	8	0.85
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	8	0.85
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	1	0.85
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	1	0.85
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	1	0.85
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE1	2	0.85
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE2	2	0.85
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE3	2	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	8	0.85
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	8	0.85
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	8	0.85
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	8	0.85
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	8	0.85
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	8	0.85
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	8	0.85
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	8	0.85
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	8	0.85
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	8	0.85
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	3	0.85
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	3	0.85
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	3	0.85
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	1	0.84
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	1	0.84
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	1	0.84
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	6	0.84
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	6	0.84
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	6	0.84
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	4	0.84
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	4	0.84
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	4	0.84
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	3	0.84
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	3	0.84
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	3	0.84
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD11	8	0.84
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD12	8	0.84
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD13	8	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	2	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	2	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	2	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	4	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	4	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	4	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	8	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	8	0.84
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	8	0.84
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	10	0.84
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	10	0.84
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	10	0.84
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	10	0.84
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	10	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	10	0.84
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	10	0.84
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	10	0.84
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	10	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE1	3	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE2	3	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE3	3	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE1	5	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE2	5	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE3	5	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE1	6	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE2	6	0.84
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE3	6	0.84
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE1	9	0.84
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE2	9	0.84
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE3	9	0.84
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	10	0.84
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	10	0.84
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	10	0.84
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	10	0.84
(2,137)	1:26:A:PHE:HB2	1:72:A:MET:HE1	5	0.84
(2,137)	1:26:A:PHE:HB2	1:72:A:MET:HE2	5	0.84
(2,137)	1:26:A:PHE:HB2	1:72:A:MET:HE3	5	0.84
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	3	0.84
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	3	0.84
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	3	0.84
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	3	0.84
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	3	0.84
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	3	0.84
(2,107)	1:22:A:ILE:HA	1:50:A:MET:HE1	7	0.84
(2,107)	1:22:A:ILE:HA	1:50:A:MET:HE2	7	0.84
(2,107)	1:22:A:ILE:HA	1:50:A:MET:HE3	7	0.84
(2,106)	1:22:A:ILE:HA	1:50:A:MET:HE1	7	0.84
(2,106)	1:22:A:ILE:HA	1:50:A:MET:HE2	7	0.84
(2,106)	1:22:A:ILE:HA	1:50:A:MET:HE3	7	0.84
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	7	0.84
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	7	0.84
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	7	0.84
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	8	0.84
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	8	0.84
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	8	0.84
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	6	0.83
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	6	0.83
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	6	0.83
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	6	0.83
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	6	0.83
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	2	0.83
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	2	0.83
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	2	0.83
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	10	0.83
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	10	0.83
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	10	0.83
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG21	9	0.82
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG22	9	0.82
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG23	9	0.82
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	8	0.8
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	8	0.8
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	8	0.8
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	6	0.8
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	6	0.8
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	6	0.8
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	6	0.8
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	6	0.8
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	6	0.8
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	9	0.79
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	9	0.79
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	9	0.79
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	1	0.78
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	1	0.78
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	1	0.78
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	2	0.78
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	2	0.78
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	2	0.78
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	8	0.78
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	8	0.78
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	8	0.78
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	3	0.78
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	3	0.78
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	3	0.78
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	2	0.78
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	2	0.78
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	2	0.78
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	2	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	2	0.78
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	2	0.78
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	1	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	1	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	1	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	1	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	1	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	1	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	1	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	1	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	1	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	4	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	4	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	4	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	4	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	4	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	4	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	4	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	4	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	4	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	6	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	6	0.77
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	6	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	6	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	6	0.77
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	6	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	6	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	6	0.77
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	6	0.77
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	7	0.76
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	7	0.76
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	7	0.76
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	2	0.76
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	2	0.76
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	2	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	2	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	2	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	2	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	2	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	2	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	2	0.76
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	3	0.76
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	3	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	3	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	3	0.76
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	3	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	3	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	3	0.76
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	3	0.76
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	4	0.75
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	4	0.75
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	4	0.75
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	1	0.75
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	1	0.75
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	1	0.75
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD11	8	0.74
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD12	8	0.74
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD13	8	0.74
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	5	0.74
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	5	0.74
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	5	0.74
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE1	5	0.74
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE2	5	0.74
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE3	5	0.74
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	5	0.74
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	5	0.74
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	5	0.74
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	10	0.73
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	10	0.73
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	10	0.73
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	10	0.73
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	10	0.73
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	10	0.73
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD1	9	0.72
(2,199)	1:36:A:ILE:HG21	1:40:A:TYR:HD2	9	0.72
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD1	9	0.72
(2,199)	1:36:A:ILE:HG22	1:40:A:TYR:HD2	9	0.72
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD1	9	0.72
(2,199)	1:36:A:ILE:HG23	1:40:A:TYR:HD2	9	0.72
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	9	0.72
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	9	0.72
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	9	0.72
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	9	0.72
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	9	0.72
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE1	1	0.72
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE2	1	0.72
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE1	1	0.72
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE2	1	0.72
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE1	1	0.72
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE2	1	0.72
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	3	0.71
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	3	0.71
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	3	0.71
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	5	0.71
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	5	0.71
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	5	0.71
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	7	0.71
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	7	0.71
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	7	0.71
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	7	0.71
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE1	10	0.71
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE2	10	0.71
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE3	10	0.71
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	2	0.71
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	2	0.71
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	2	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	1	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	1	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	1	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	1	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	1	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	1	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	2	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	2	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	2	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	2	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	2	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	2	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	3	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	3	0.71
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	3	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	3	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	3	0.71
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	1	0.7
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	1	0.7
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	1	0.7
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE1	5	0.7
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE2	5	0.7
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE1	5	0.7
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE2	5	0.7
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE1	5	0.7
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE2	5	0.7
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE1	8	0.7
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE2	8	0.7
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE1	8	0.7
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE2	8	0.7
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE1	8	0.7
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE2	8	0.7
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE1	9	0.7
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE2	9	0.7
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE1	9	0.7
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE2	9	0.7
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE1	9	0.7
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE2	9	0.7
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	7	0.7
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	7	0.7
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	7	0.7
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	7	0.7
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	7	0.7
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	7	0.7
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	8	0.7
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	8	0.7
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	8	0.7
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	8	0.7
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	8	0.7
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	8	0.7
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	7	0.69
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	7	0.69
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	7	0.69
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	6	0.69
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	6	0.69
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	6	0.69
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	6	0.69
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	9	0.69
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	9	0.69
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	9	0.69
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	8	0.69
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	8	0.69
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	8	0.69
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	3	0.69
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	3	0.69
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	3	0.69
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	3	0.69
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	3	0.69
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	3	0.69
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	10	0.68
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	10	0.68
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	10	0.68
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	4	0.68
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	4	0.68
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	4	0.68
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	4	0.68
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	1	0.68
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	1	0.68
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	1	0.68
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	1	0.68
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	1	0.68
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	1	0.68
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	3	0.68
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	3	0.68
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	3	0.68
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	3	0.68
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	3	0.68
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	3	0.68
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	6	0.68
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	6	0.68
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	6	0.68
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	6	0.68
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	6	0.68
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	6	0.68
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	8	0.68
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	8	0.68
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	8	0.68
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	8	0.68
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	8	0.68
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	8	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	8	0.68
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	8	0.68
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	8	0.68
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	9	0.68
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	9	0.68
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	9	0.68
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	9	0.68
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	9	0.68
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	9	0.68
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	9	0.68
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	9	0.68
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	9	0.68
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	5	0.67
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	5	0.67
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	5	0.67
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	2	0.67
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	2	0.67
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	2	0.67
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	6	0.67
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	6	0.67
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	6	0.67
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	9	0.67
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	9	0.67
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	9	0.67
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	9	0.67
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	9	0.67
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	1	0.67
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	1	0.67
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	1	0.67
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	1	0.67
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	1	0.67
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	1	0.67
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	10	0.67
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	10	0.67
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	10	0.67
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	10	0.67
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	10	0.67
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	10	0.67
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	8	0.66
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	8	0.66
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	8	0.66
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	8	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	8	0.66
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	8	0.66
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	8	0.66
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	8	0.66
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	8	0.66
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	9	0.66
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	9	0.66
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	9	0.66
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	6	0.66
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	6	0.66
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	6	0.66
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	6	0.66
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	6	0.66
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	6	0.66
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	10	0.66
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	10	0.66
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	10	0.66
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	10	0.66
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	10	0.66
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	10	0.66
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	10	0.66
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	10	0.66
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	10	0.66
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	5	0.65
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	5	0.65
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	5	0.65
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	7	0.65
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	7	0.65
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	7	0.65
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	10	0.65
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	10	0.65
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	5	0.65
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	5	0.65
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	5	0.65
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	5	0.65
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	5	0.65
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	5	0.65
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	5	0.65
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	5	0.65
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	5	0.65
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	5	0.64
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	5	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	5	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	1	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	1	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	3	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	3	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	5	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	5	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	6	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	6	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	7	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	7	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	8	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	8	0.64
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE1	9	0.64
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE2	9	0.64
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE3	9	0.64
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	1	0.64
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	1	0.64
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	1	0.64
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	1	0.64
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	2	0.64
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	2	0.64
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	2	0.64
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	4	0.64
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	4	0.64
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	4	0.64
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	6	0.64
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	6	0.64
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	6	0.64
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	2	0.64
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	2	0.64
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	2	0.64
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	2	0.64
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	2	0.64
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	2	0.64
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	7	0.64
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	7	0.64
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	7	0.64
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	7	0.64
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	7	0.64
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	7	0.64
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	4	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	4	0.63
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	1	0.63
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	1	0.63
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	1	0.63
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	6	0.63
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	6	0.63
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	6	0.63
(2,10)	1:1:A:SER:HB2	1:3:A:LYS:H	5	0.63
(2,10)	1:1:A:SER:HB3	1:3:A:LYS:H	5	0.63
(2,10)	1:1:A:SER:HB2	1:3:A:LYS:H	8	0.63
(2,10)	1:1:A:SER:HB3	1:3:A:LYS:H	8	0.63
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	3	0.63
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	3	0.63
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	3	0.63
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	1	0.63
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	1	0.63
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	1	0.63
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	7	0.63
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	7	0.63
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	7	0.63
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	8	0.63
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	8	0.63
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	8	0.63
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	10	0.63
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	10	0.63
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	10	0.63
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	10	0.63
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	10	0.63
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	10	0.63
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	7	0.63
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	7	0.63
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	7	0.63
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	7	0.63
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	7	0.63
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	7	0.63
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	9	0.63
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	9	0.63
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	9	0.63
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	9	0.63
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	9	0.63
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	9	0.63
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	6	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	6	0.63
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	6	0.63
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	4	0.62
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	4	0.62
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	5	0.62
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	5	0.62
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	2	0.62
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	2	0.62
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	1	0.62
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	1	0.62
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	4	0.62
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	4	0.62
(2,49)	1:5:A:VAL:HG21	1:7:A:SER:HA	4	0.62
(2,49)	1:5:A:VAL:HG22	1:7:A:SER:HA	4	0.62
(2,49)	1:5:A:VAL:HG23	1:7:A:SER:HA	4	0.62
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	9	0.62
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	9	0.62
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	9	0.62
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	9	0.62
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	9	0.62
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	9	0.62
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	9	0.62
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	9	0.62
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	9	0.62
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	3	0.62
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	3	0.62
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	3	0.62
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	1	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	1	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	3	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	3	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	7	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	7	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	8	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	8	0.61
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE1	1	0.61
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE2	1	0.61
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE3	1	0.61
(2,10)	1:1:A:SER:HB2	1:3:A:LYS:H	2	0.61
(2,10)	1:1:A:SER:HB3	1:3:A:LYS:H	2	0.61
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB1	8	0.61
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB2	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2541)	1:26:A:PHE:HD1	1:27:A:ALA:HB3	8	0.61
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB1	8	0.61
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB2	8	0.61
(1,2541)	1:26:A:PHE:HD2	1:27:A:ALA:HB3	8	0.61
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	7	0.61
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	7	0.61
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	7	0.61
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	10	0.61
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	10	0.61
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	10	0.61
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	1	0.61
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	1	0.61
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	1	0.61
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	2	0.6
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	2	0.6
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	6	0.6
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	6	0.6
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD1	10	0.6
(2,267)	1:51:A:VAL:H	1:52:A:PHE:HD2	10	0.6
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD1	9	0.6
(2,257)	1:48:A:THR:HA	1:52:A:PHE:HD2	9	0.6
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	2	0.6
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	2	0.6
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	3	0.6
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	3	0.6
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	2	0.6
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	2	0.6
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	2	0.6
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	2	0.6
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	4	0.6
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	4	0.6
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	1	0.6
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	1	0.6
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	1	0.6
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD1	1	0.6
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD2	1	0.6
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD1	1	0.6
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD2	1	0.6
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD1	1	0.6
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD2	1	0.6
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	7	0.59
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	2	0.59
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	2	0.59
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	9	0.59
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	9	0.59
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	3	0.59
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	3	0.59
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	9	0.59
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	9	0.59
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	8	0.58
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	8	0.58
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	6	0.58
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	6	0.58
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	7	0.58
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	7	0.58
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	8	0.58
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	8	0.58
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	10	0.58
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	10	0.58
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	1	0.58
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	1	0.58
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	7	0.58
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	7	0.58
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	7	0.58
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	7	0.58
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	7	0.58
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	7	0.58
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	7	0.58
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	7	0.58
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	10	0.58
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	10	0.58
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	10	0.58
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG11	6	0.58
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG12	6	0.58
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG13	6	0.58
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	6	0.57
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	6	0.57
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	10	0.57
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	10	0.57
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	10	0.57
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	9	0.57
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	9	0.57
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE2	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE3	2	0.57
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	5	0.57
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	5	0.57
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	6	0.57
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	6	0.57
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	9	0.57
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	9	0.57
(2,210)	1:40:A:TYR:HE1	1:52:A:PHE:HB3	10	0.57
(2,210)	1:40:A:TYR:HE2	1:52:A:PHE:HB3	10	0.57
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	1	0.57
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	1	0.57
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	4	0.57
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	4	0.57
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	5	0.57
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	5	0.57
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	1	0.57
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	1	0.57
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	6	0.57
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	6	0.57
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	9	0.57
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	9	0.57
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	6	0.57
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	6	0.57
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	2	0.57
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	2	0.57
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	2	0.57
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	4	0.57
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	4	0.57
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	4	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG11	2	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG12	2	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG13	2	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG11	3	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG12	3	0.57
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG13	3	0.57
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	5	0.56
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	5	0.56
(2,265)	1:50:A:MET:HE1	1:102:A:TYR:HE1	7	0.56
(2,265)	1:50:A:MET:HE1	1:102:A:TYR:HE2	7	0.56
(2,265)	1:50:A:MET:HE2	1:102:A:TYR:HE1	7	0.56
(2,265)	1:50:A:MET:HE2	1:102:A:TYR:HE2	7	0.56
(2,265)	1:50:A:MET:HE3	1:102:A:TYR:HE1	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:50:A:MET:HE3	1:102:A:TYR:HE2	7	0.56
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE2	5	0.56
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE3	5	0.56
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE2	4	0.56
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE3	4	0.56
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE2	9	0.56
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE3	9	0.56
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	3	0.56
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	3	0.56
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE2	1	0.56
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE3	1	0.56
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE2	3	0.56
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE3	3	0.56
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE2	8	0.56
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE3	8	0.56
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	4	0.56
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	4	0.56
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	5	0.56
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	5	0.56
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	7	0.56
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	7	0.56
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	10	0.56
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	10	0.56
(2,32)	1:3:A:LYS:HD2	1:53:A:ILE:HA	10	0.56
(2,32)	1:3:A:LYS:HD3	1:53:A:ILE:HA	10	0.56
(2,29)	1:2:A:VAL:H	1:54:A:LYS:HE2	4	0.56
(2,29)	1:2:A:VAL:H	1:54:A:LYS:HE3	4	0.56
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	6	0.56
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	6	0.56
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	6	0.56
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD1	9	0.56
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD2	9	0.56
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD1	9	0.56
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD2	9	0.56
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD1	9	0.56
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD2	9	0.56
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	4	0.56
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	4	0.56
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	4	0.56
(1,572)	1:20:A:LEU:HB2	1:77:A:VAL:HG11	5	0.56
(1,572)	1:20:A:LEU:HB2	1:77:A:VAL:HG12	5	0.56
(1,572)	1:20:A:LEU:HB2	1:77:A:VAL:HG13	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,572)	1:20:A:LEU:HB3	1:77:A:VAL:HG11	5	0.56
(1,572)	1:20:A:LEU:HB3	1:77:A:VAL:HG12	5	0.56
(1,572)	1:20:A:LEU:HB3	1:77:A:VAL:HG13	5	0.56
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	1	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	1	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	2	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	2	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	3	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	3	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	9	0.55
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	9	0.55
(2,258)	1:48:A:THR:HB	1:49:A:LYS:HD2	6	0.55
(2,258)	1:48:A:THR:HB	1:49:A:LYS:HD3	6	0.55
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE2	8	0.55
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE3	8	0.55
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	5	0.55
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	5	0.55
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	10	0.55
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	10	0.55
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE2	1	0.55
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE3	1	0.55
(2,163)	1:28:A:GLU:HG2	1:29:A:TRP:H	3	0.55
(2,163)	1:28:A:GLU:HG3	1:29:A:TRP:H	3	0.55
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	9	0.55
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	9	0.55
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	9	0.55
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	9	0.55
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	2	0.55
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	2	0.55
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE2	7	0.55
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE3	7	0.55
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	2	0.55
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	2	0.55
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	8	0.55
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	8	0.55
(2,15)	1:1:A:SER:HB2	1:52:A:PHE:H	4	0.55
(2,15)	1:1:A:SER:HB3	1:52:A:PHE:H	4	0.55
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	4	0.55
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	4	0.55
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	2	0.55
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	2	0.55
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	2	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	5	0.55
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	5	0.55
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	5	0.55
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	6	0.55
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	6	0.55
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	6	0.55
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	7	0.55
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	7	0.55
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	7	0.55
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	8	0.55
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	8	0.55
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	8	0.55
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	9	0.55
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	9	0.55
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	9	0.55
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	10	0.55
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	10	0.55
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	10	0.55
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	8	0.55
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	8	0.55
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	8	0.55
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	9	0.55
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	9	0.55
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	9	0.55
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	6	0.55
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	6	0.55
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	6	0.55
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	6	0.55
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	6	0.55
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	6	0.55
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	6	0.55
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	6	0.55
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	6	0.55
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	4	0.55
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	4	0.55
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	4	0.55
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	4	0.55
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	4	0.55
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	4	0.55
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	10	0.55
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	10	0.55
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	10	0.55
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	10	0.55
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	10	0.55
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG11	8	0.55
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG12	8	0.55
(1,606)	1:21:A:VAL:HA	1:51:A:VAL:HG13	8	0.55
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	4	0.54
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	4	0.54
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	4	0.54
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	4	0.54
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	4	0.54
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	4	0.54
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	5	0.54
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	5	0.54
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	5	0.54
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	10	0.54
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	10	0.54
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	10	0.54
(1,2475)	1:101:A:LYS:HE2	1:102:A:TYR:HE1	9	0.54
(1,2475)	1:101:A:LYS:HE2	1:102:A:TYR:HE2	9	0.54
(1,2475)	1:101:A:LYS:HE3	1:102:A:TYR:HE1	9	0.54
(1,2475)	1:101:A:LYS:HE3	1:102:A:TYR:HE2	9	0.54
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	3	0.54
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	3	0.54
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	3	0.54
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG21	4	0.54
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG22	4	0.54
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG23	4	0.54
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	1	0.53
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	1	0.53
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	1	0.53
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	1	0.53
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	1	0.53
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	1	0.53
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	1	0.53
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	1	0.53
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	1	0.53
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	1	0.53
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	1	0.53
(2,74)	1:11:A:PHE:HD1	1:12:A:ASP:HB2	3	0.53
(2,74)	1:11:A:PHE:HD2	1:12:A:ASP:HB2	3	0.53
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	6	0.53
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	6	0.53
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	2	0.53
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	2	0.53
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	2	0.53
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	2	0.53
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	2	0.53
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	2	0.53
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG21	7	0.53
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG22	7	0.53
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG23	7	0.53
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG21	9	0.53
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG22	9	0.53
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG23	9	0.53
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	9	0.53
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	9	0.53
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	9	0.53
(2,326)	1:69:A:ILE:HG21	1:72:A:MET:HA	9	0.52
(2,326)	1:69:A:ILE:HG22	1:72:A:MET:HA	9	0.52
(2,326)	1:69:A:ILE:HG23	1:72:A:MET:HA	9	0.52
(1,2423)	1:99:A:ILE:HG21	1:100:A:GLU:H	5	0.52
(1,2423)	1:99:A:ILE:HG22	1:100:A:GLU:H	5	0.52
(1,2423)	1:99:A:ILE:HG23	1:100:A:GLU:H	5	0.52
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	4	0.52
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	4	0.52
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	4	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG21	1	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG22	1	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG23	1	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG21	5	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG22	5	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG23	5	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG21	10	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG22	10	0.52
(1,607)	1:21:A:VAL:HA	1:51:A:VAL:HG23	10	0.52
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	2	0.52
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	2	0.52
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	2	0.52
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	3	0.52
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	3	0.52
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	3	0.52
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	10	0.51
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	10	0.51
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	8	0.51
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	8	0.51
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE2	2	0.51
(2,215)	1:42:A:GLU:H	1:45:A:LYS:HE3	2	0.51
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	7	0.51
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	7	0.51
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	4	0.51
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	4	0.51
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	4	0.51
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	9	0.51
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	9	0.51
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	9	0.51
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	8	0.5
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	8	0.5
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	9	0.5
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	9	0.5
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	9	0.5
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	2	0.5
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	2	0.5
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	2	0.5
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	9	0.5
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	9	0.5
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD2	4	0.5
(2,140)	1:26:A:PHE:HE1	1:54:A:LYS:HD3	4	0.5
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD2	4	0.5
(2,140)	1:26:A:PHE:HE2	1:54:A:LYS:HD3	4	0.5
(2,10)	1:1:A:SER:HB2	1:3:A:LYS:H	4	0.5
(2,10)	1:1:A:SER:HB3	1:3:A:LYS:H	4	0.5
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	10	0.5
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	10	0.5
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	10	0.5
(1,2199)	1:88:A:LEU:HD11	1:88:A:LEU:H	5	0.5
(1,2199)	1:88:A:LEU:HD12	1:88:A:LEU:H	5	0.5
(1,2199)	1:88:A:LEU:HD13	1:88:A:LEU:H	5	0.5
(1,2197)	1:88:A:LEU:HD11	1:89:A:GLY:H	4	0.5
(1,2197)	1:88:A:LEU:HD12	1:89:A:GLY:H	4	0.5
(1,2197)	1:88:A:LEU:HD13	1:89:A:GLY:H	4	0.5
(1,2197)	1:88:A:LEU:HD21	1:89:A:GLY:H	4	0.5
(1,2197)	1:88:A:LEU:HD22	1:89:A:GLY:H	4	0.5
(1,2197)	1:88:A:LEU:HD23	1:89:A:GLY:H	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	2	0.5
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	2	0.5
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	2	0.5
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	2	0.5
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	2	0.5
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	2	0.5
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	2	0.5
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	2	0.5
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	2	0.5
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	2	0.5
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	2	0.5
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	2	0.5
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	2	0.5
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	2	0.5
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	2	0.5
(1,1631)	1:63:A:VAL:HG11	1:66:A:LYS:HG2	7	0.5
(1,1631)	1:63:A:VAL:HG11	1:66:A:LYS:HG3	7	0.5
(1,1631)	1:63:A:VAL:HG12	1:66:A:LYS:HG2	7	0.5
(1,1631)	1:63:A:VAL:HG12	1:66:A:LYS:HG3	7	0.5
(1,1631)	1:63:A:VAL:HG13	1:66:A:LYS:HG2	7	0.5
(1,1631)	1:63:A:VAL:HG13	1:66:A:LYS:HG3	7	0.5
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	8	0.5
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	8	0.5
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	8	0.5
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	1	0.5
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	1	0.5
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	1	0.5
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	2	0.5
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	2	0.5
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	2	0.5
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	5	0.5
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	5	0.5
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	5	0.5
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	6	0.5
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	6	0.5
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	6	0.5
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	2	0.49
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	2	0.49
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	2	0.49
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	4	0.49
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	4	0.49
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	10	0.49
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	10	0.49
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	10	0.49
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	3	0.49
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	3	0.49
(2,82)	1:12:A:ASP:HB2	1:66:A:LYS:HD2	8	0.49
(2,82)	1:12:A:ASP:HB2	1:66:A:LYS:HD3	8	0.49
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	3	0.49
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	3	0.49
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	3	0.49
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	3	0.49
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	3	0.49
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	3	0.49
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	3	0.49
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	3	0.49
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	3	0.49
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	6	0.49
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	6	0.49
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	6	0.49
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	3	0.49
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	3	0.49
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	3	0.49
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	6	0.49
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	6	0.49
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	6	0.49
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	7	0.49
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	7	0.49
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	7	0.49
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	7	0.49
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	7	0.49
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	7	0.49
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	8	0.49
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	8	0.49
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	8	0.49
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	10	0.49
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	10	0.49
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	10	0.49
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	3	0.49
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	3	0.49
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	3	0.49
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	3	0.49
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	3	0.49
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	3	0.49
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	3	0.49
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	3	0.49
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	3	0.49
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	3	0.49
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	3	0.49
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	3	0.49
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	3	0.49
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	3	0.49
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	3	0.49
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	3	0.49
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	3	0.49
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	9	0.48
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	9	0.48
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	9	0.48
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	10	0.48
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	10	0.48
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	10	0.48
(2,229)	1:44:A:SER:HG	1:45:A:LYS:HD2	6	0.48
(2,229)	1:44:A:SER:HG	1:45:A:LYS:HD3	6	0.48
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	1	0.48
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	1	0.48
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	1	0.48
(1,2388)	1:98:A:LEU:HD21	1:99:A:ILE:HA	5	0.48
(1,2388)	1:98:A:LEU:HD22	1:99:A:ILE:HA	5	0.48
(1,2388)	1:98:A:LEU:HD23	1:99:A:ILE:HA	5	0.48
(1,1959)	1:77:A:VAL:HG11	1:102:A:TYR:HB2	5	0.48
(1,1959)	1:77:A:VAL:HG12	1:102:A:TYR:HB2	5	0.48
(1,1959)	1:77:A:VAL:HG13	1:102:A:TYR:HB2	5	0.48
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	5	0.48
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	5	0.48
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	5	0.48
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	9	0.48
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	9	0.48
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	9	0.48
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	2	0.48
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	2	0.48
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	2	0.48
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG11	9	0.48
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG12	9	0.48
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG13	9	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	9	0.48
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	9	0.48
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	9	0.48
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD11	6	0.47
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD12	6	0.47
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD13	6	0.47
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE1	2	0.47
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE2	2	0.47
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE1	5	0.47
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE2	5	0.47
(2,109)	1:22:A:ILE:H	1:50:A:MET:HE3	5	0.47
(1,2551)	1:27:A:ALA:HB1	1:30:A:CYS:H	4	0.47
(1,2551)	1:27:A:ALA:HB2	1:30:A:CYS:H	4	0.47
(1,2551)	1:27:A:ALA:HB3	1:30:A:CYS:H	4	0.47
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB1	5	0.47
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB2	5	0.47
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB3	5	0.47
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	8	0.47
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	8	0.47
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	8	0.47
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	4	0.47
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	4	0.47
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	4	0.47
(1,747)	1:23:A:VAL:HG21	1:53:A:ILE:HG12	1	0.47
(1,747)	1:23:A:VAL:HG22	1:53:A:ILE:HG12	1	0.47
(1,747)	1:23:A:VAL:HG23	1:53:A:ILE:HG12	1	0.47
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	8	0.47
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	8	0.47
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	8	0.47
(1,576)	1:20:A:LEU:HD11	1:78:A:TYR:H	10	0.47
(1,576)	1:20:A:LEU:HD12	1:78:A:TYR:H	10	0.47
(1,576)	1:20:A:LEU:HD13	1:78:A:TYR:H	10	0.47
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	9	0.47
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	9	0.47
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	9	0.47
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	9	0.47
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	9	0.47
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	9	0.47
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	9	0.47
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	9	0.47
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	9	0.47
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	9	0.47
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	9	0.47
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	9	0.47
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	9	0.47
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	9	0.47
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	9	0.47
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	9	0.47
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	9	0.47
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	3	0.47
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	3	0.47
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	3	0.47
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	3	0.47
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	3	0.47
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	3	0.47
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	7	0.46
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	7	0.46
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	7	0.46
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	7	0.46
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	8	0.46
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	8	0.46
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	8	0.46
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	8	0.46
(1,2546)	1:27:A:ALA:HB1	1:29:A:TRP:HD1	3	0.46
(1,2546)	1:27:A:ALA:HB2	1:29:A:TRP:HD1	3	0.46
(1,2546)	1:27:A:ALA:HB3	1:29:A:TRP:HD1	3	0.46
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD1	8	0.46
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD2	8	0.46
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD1	8	0.46
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD2	8	0.46
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD1	8	0.46
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD2	8	0.46
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	6	0.46
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	6	0.46
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	6	0.46
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	9	0.46
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	9	0.46
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	9	0.46
(1,1631)	1:63:A:VAL:HG11	1:66:A:LYS:HG2	8	0.46
(1,1631)	1:63:A:VAL:HG11	1:66:A:LYS:HG3	8	0.46
(1,1631)	1:63:A:VAL:HG12	1:66:A:LYS:HG2	8	0.46
(1,1631)	1:63:A:VAL:HG12	1:66:A:LYS:HG3	8	0.46
(1,1631)	1:63:A:VAL:HG13	1:66:A:LYS:HG2	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1631)	1:63:A:VAL:HG13	1:66:A:LYS:HG3	8	0.46
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	2	0.46
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	2	0.46
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	2	0.46
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	3	0.46
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	3	0.46
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	3	0.46
(1,747)	1:23:A:VAL:HG21	1:53:A:ILE:HG12	9	0.46
(1,747)	1:23:A:VAL:HG22	1:53:A:ILE:HG12	9	0.46
(1,747)	1:23:A:VAL:HG23	1:53:A:ILE:HG12	9	0.46
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	5	0.46
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	5	0.46
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	5	0.46
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	9	0.46
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	9	0.46
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	9	0.46
(1,591)	1:20:A:LEU:H	1:20:A:LEU:HD21	5	0.46
(1,591)	1:20:A:LEU:H	1:20:A:LEU:HD22	5	0.46
(1,591)	1:20:A:LEU:H	1:20:A:LEU:HD23	5	0.46
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	1	0.46
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	1	0.46
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	1	0.46
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	2	0.46
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	2	0.46
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	2	0.46
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	3	0.46
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	3	0.46
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	3	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	2	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	2	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	2	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	3	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	3	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	3	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	6	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	6	0.46
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	6	0.46
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	2	0.46
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	2	0.46
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	2	0.46
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	2	0.46
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	2	0.46
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	2	0.46
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	2	0.46
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	2	0.46
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	6	0.46
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	6	0.46
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	6	0.46
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	6	0.46
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	6	0.46
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	6	0.46
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	6	0.46
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	6	0.46
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	6	0.46
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	2	0.46
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	2	0.46
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	2	0.46
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	2	0.46
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	2	0.46
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	2	0.46
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	2	0.46
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	2	0.46
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	2	0.46
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	6	0.46
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	6	0.46
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	6	0.46
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	6	0.46
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	6	0.46
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	6	0.46
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	6	0.46
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	6	0.46
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	6	0.46
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	7	0.46
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	7	0.46
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	7	0.46
(2,328)	1:69:A:ILE:HG21	1:72:A:MET:HB2	4	0.45
(2,328)	1:69:A:ILE:HG22	1:72:A:MET:HB2	4	0.45
(2,328)	1:69:A:ILE:HG23	1:72:A:MET:HB2	4	0.45
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE1	8	0.45
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE2	8	0.45
(2,193)	1:29:A:TRP:HZ3	1:72:A:MET:HE3	8	0.45
(1,2475)	1:101:A:LYS:HE2	1:102:A:TYR:HE1	8	0.45
(1,2475)	1:101:A:LYS:HE2	1:102:A:TYR:HE2	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2475)	1:101:A:LYS:HE3	1:102:A:TYR:HE1	8	0.45
(1,2475)	1:101:A:LYS:HE3	1:102:A:TYR:HE2	8	0.45
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG21	4	0.45
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG22	4	0.45
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG23	4	0.45
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	2	0.45
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	2	0.45
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	2	0.45
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	4	0.45
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	4	0.45
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	4	0.45
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	5	0.45
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	5	0.45
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	5	0.45
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	6	0.45
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	6	0.45
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	6	0.45
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	9	0.45
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	9	0.45
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	9	0.45
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	9	0.45
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	9	0.45
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	9	0.45
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	6	0.45
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	6	0.45
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	6	0.45
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	6	0.45
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	6	0.45
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	6	0.45
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	5	0.45
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	5	0.45
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	5	0.45
(1,718)	1:23:A:VAL:HG11	1:53:A:ILE:HG13	1	0.45
(1,718)	1:23:A:VAL:HG12	1:53:A:ILE:HG13	1	0.45
(1,718)	1:23:A:VAL:HG13	1:53:A:ILE:HG13	1	0.45
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	2	0.45
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	2	0.45
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	2	0.45
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	6	0.45
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	6	0.45
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	6	0.45
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	7	0.45
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	7	0.45
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	8	0.45
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	8	0.45
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	8	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	5	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	5	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	5	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	5	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	5	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	5	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	5	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	5	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	5	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	8	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	8	0.45
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	8	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	8	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	8	0.45
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	8	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	8	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	8	0.45
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	8	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	5	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	5	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	5	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	5	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	5	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	5	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	5	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	5	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	5	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	8	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	8	0.45
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	8	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	8	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	8	0.45
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	8	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	8	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	8	0.45
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	8	0.45
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	6	0.44
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	6	0.44
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	6	0.44
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	6	0.44
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	6	0.44
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB1	4	0.44
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB2	4	0.44
(2,238)	1:46:A:THR:HG21	1:104:A:ALA:HB3	4	0.44
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB1	4	0.44
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB2	4	0.44
(2,238)	1:46:A:THR:HG22	1:104:A:ALA:HB3	4	0.44
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB1	4	0.44
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB2	4	0.44
(2,238)	1:46:A:THR:HG23	1:104:A:ALA:HB3	4	0.44
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	6	0.44
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	6	0.44
(2,79)	1:12:A:ASP:HB3	1:66:A:LYS:HD2	8	0.44
(2,79)	1:12:A:ASP:HB3	1:66:A:LYS:HD3	8	0.44
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	2	0.44
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	2	0.44
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	2	0.44
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	4	0.44
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	4	0.44
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	4	0.44
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	6	0.44
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	6	0.44
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	6	0.44
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG21	8	0.44
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG22	8	0.44
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG23	8	0.44
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	3	0.44
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	3	0.44
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	3	0.44
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	7	0.44
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	7	0.44
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	7	0.44
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	8	0.44
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	8	0.44
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	8	0.44
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	9	0.44
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	9	0.44
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	10	0.44
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	10	0.44
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	10	0.44
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	8	0.44
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	8	0.44
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	8	0.44
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	2	0.44
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	2	0.44
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	2	0.44
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	2	0.44
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	2	0.44
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	2	0.44
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	2	0.44
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	2	0.44
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	2	0.44
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	6	0.44
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	6	0.44
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	6	0.44
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	6	0.44
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	6	0.44
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	6	0.44
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	1	0.44
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	1	0.44
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	1	0.44
(1,1336)	1:46:A:THR:HG21	1:47:A:TYR:H	9	0.44
(1,1336)	1:46:A:THR:HG22	1:47:A:TYR:H	9	0.44
(1,1336)	1:46:A:THR:HG23	1:47:A:TYR:H	9	0.44
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	5	0.44
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	5	0.44
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	5	0.44
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	9	0.44
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	9	0.44
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	9	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	1	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	1	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	1	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	10	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	10	0.44
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	10	0.44
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG21	3	0.44
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG22	3	0.44
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG23	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	10	0.44
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	10	0.44
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	10	0.44
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	10	0.44
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	10	0.44
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	10	0.44
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	10	0.44
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	10	0.44
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	10	0.44
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	10	0.44
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	10	0.44
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	10	0.44
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	10	0.44
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	10	0.44
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	10	0.44
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	10	0.44
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	10	0.44
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	10	0.44
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	1	0.43
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	1	0.43
(2,209)	1:40:A:TYR:HD1	1:43:A:CYS:H	2	0.43
(2,209)	1:40:A:TYR:HD2	1:43:A:CYS:H	2	0.43
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	3	0.43
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	3	0.43
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	10	0.43
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	10	0.43
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	10	0.43
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	10	0.43
(1,2310)	1:95:A:LEU:HD21	1:95:A:LEU:HB3	1	0.43
(1,2310)	1:95:A:LEU:HD22	1:95:A:LEU:HB3	1	0.43
(1,2310)	1:95:A:LEU:HD23	1:95:A:LEU:HB3	1	0.43
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	7	0.43
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	7	0.43
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	7	0.43
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	9	0.43
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	9	0.43
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	9	0.43
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	3	0.43
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	3	0.43
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	3	0.43
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	5	0.43
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	5	0.43
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	8	0.43
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	8	0.43
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	8	0.43
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	8	0.43
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	8	0.43
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	8	0.43
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	7	0.43
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	7	0.43
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	7	0.43
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	4	0.43
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	4	0.43
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	4	0.43
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG11	8	0.43
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG12	8	0.43
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG13	8	0.43
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	4	0.43
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	4	0.43
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	4	0.43
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG21	5	0.43
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG22	5	0.43
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG23	5	0.43
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	7	0.43
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	7	0.43
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	7	0.43
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	7	0.43
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	7	0.43
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	7	0.43
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	7	0.43
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	7	0.43
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	7	0.43
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	7	0.43
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	7	0.43
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	7	0.43
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	7	0.43
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	7	0.43
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	7	0.43
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	7	0.43
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	7	0.43
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	7	0.43
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	2	0.43
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	2	0.43
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	4	0.43
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	4	0.43
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	4	0.43
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	6	0.42
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	6	0.42
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	8	0.42
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	8	0.42
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	9	0.42
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	9	0.42
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG21	6	0.42
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG22	6	0.42
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG23	6	0.42
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	1	0.42
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	1	0.42
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	1	0.42
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	2	0.42
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	2	0.42
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	2	0.42
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	4	0.42
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	4	0.42
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	4	0.42
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	7	0.42
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	7	0.42
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	7	0.42
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	7	0.42
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	7	0.42
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	7	0.42
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	7	0.42
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	7	0.42
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	7	0.42
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	6	0.42
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	6	0.42
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	6	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	2	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	2	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	2	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	8	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	8	0.42
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	8	0.42
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	3	0.42
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	3	0.42
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	6	0.42
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	6	0.42
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	6	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	6	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	6	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	6	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	7	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	7	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	7	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	8	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	8	0.42
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	8	0.42
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	4	0.42
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	4	0.42
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	4	0.42
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	1	0.42
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	1	0.42
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	1	0.42
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	1	0.42
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	1	0.42
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	1	0.42
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	1	0.42
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	1	0.42
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	1	0.42
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	1	0.42
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	1	0.42
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	1	0.42
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	1	0.42
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	1	0.42
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	1	0.42
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	1	0.42
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	1	0.42
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	1	0.42
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	8	0.42
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	8	0.42
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	8	0.42
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	9	0.41
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	9	0.41
(2,371)	1:76:A:LYS:HG2	1:78:A:TYR:H	9	0.41
(2,371)	1:76:A:LYS:HG3	1:78:A:TYR:H	9	0.41
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	1	0.41
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	1	0.41
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	2	0.41
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	2	0.41
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	2	0.41
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	9	0.41
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	9	0.41
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	10	0.41
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	10	0.41
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	7	0.41
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	7	0.41
(2,127)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	7	0.41
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD11	7	0.41
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD12	7	0.41
(2,126)	1:25:A:PHE:HZ	1:69:A:ILE:HD13	7	0.41
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	1	0.41
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	1	0.41
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	3	0.41
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	3	0.41
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	7	0.41
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	7	0.41
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	3	0.41
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	3	0.41
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	3	0.41
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	6	0.41
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	6	0.41
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	6	0.41
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	9	0.41
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	9	0.41
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	9	0.41
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	4	0.41
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	4	0.41
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	4	0.41
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	7	0.41
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	7	0.41
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	7	0.41
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	3	0.41
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	3	0.41
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	3	0.41
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	5	0.41
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	5	0.41
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	3	0.41
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	3	0.41
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	3	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	1	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	1	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	1	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	4	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	4	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	4	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	5	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	5	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	5	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	8	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	8	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	8	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	10	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	10	0.41
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	10	0.41
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	8	0.41
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	8	0.41
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	8	0.41
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	10	0.41
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	10	0.41
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	10	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	8	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	8	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	8	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	9	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	9	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	9	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	10	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	10	0.41
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	10	0.41
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	3	0.41
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	3	0.41
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	3	0.41
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	3	0.41
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	3	0.41
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	3	0.41
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	10	0.41
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	10	0.41
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD11	7	0.41
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD12	7	0.41
(1,555)	1:20:A:LEU:HA	1:20:A:LEU:HD13	7	0.41
(1,424)	1:15:A:ILE:HG21	1:78:A:TYR:HB3	4	0.41
(1,424)	1:15:A:ILE:HG22	1:78:A:TYR:HB3	4	0.41
(1,424)	1:15:A:ILE:HG23	1:78:A:TYR:HB3	4	0.41
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	2	0.41
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	2	0.41
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	2	0.41
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	9	0.41
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	9	0.41
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	9	0.41
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	5	0.41
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	5	0.41
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	5	0.41
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	8	0.41
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	8	0.41
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	8	0.41
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	2	0.41
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	2	0.41
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	2	0.41
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	10	0.41
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	10	0.41
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	10	0.41
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	1	0.4
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	1	0.4
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	7	0.4
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	7	0.4
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	7	0.4
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	3	0.4
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	3	0.4
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	3	0.4
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	4	0.4
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	4	0.4
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	8	0.4
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	8	0.4
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	8	0.4
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	2	0.4
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	2	0.4
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	2	0.4
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	8	0.4
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	8	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	8	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	2	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	2	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	2	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	5	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	5	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	5	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	8	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	8	0.4
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	8	0.4
(1,2172)	1:87:A:LEU:HD11	1:91:A:ASN:HB2	6	0.4
(1,2172)	1:87:A:LEU:HD12	1:91:A:ASN:HB2	6	0.4
(1,2172)	1:87:A:LEU:HD13	1:91:A:ASN:HB2	6	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	2	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	2	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	2	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	3	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	3	0.4
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	3	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD11	2	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD12	2	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD13	2	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD11	3	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD12	3	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD13	3	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD11	7	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD12	7	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD13	7	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD11	8	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD12	8	0.4
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD13	8	0.4
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG21	9	0.4
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG22	9	0.4
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG23	9	0.4
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	4	0.4
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	4	0.4
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	4	0.4
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	4	0.4
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	4	0.4
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	4	0.4
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	5	0.4
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	5	0.4
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	5	0.4
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	5	0.4
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	5	0.4
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	4	0.4
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	4	0.4
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	4	0.4
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	1	0.4
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	1	0.4
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	1	0.4
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	5	0.4
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	5	0.4
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	5	0.4
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB1	9	0.4
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB2	9	0.4
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB3	9	0.4
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	1	0.4
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	1	0.4
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	1	0.4
(1,652)	1:22:A:ILE:HD11	1:23:A:VAL:H	8	0.4
(1,652)	1:22:A:ILE:HD12	1:23:A:VAL:H	8	0.4
(1,652)	1:22:A:ILE:HD13	1:23:A:VAL:H	8	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	1	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	1	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	1	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	10	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	10	0.4
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	10	0.4
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	1	0.4
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	1	0.4
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	1	0.4
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	7	0.4
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	7	0.4
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	7	0.4
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	10	0.4
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	10	0.4
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	10	0.4
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	1	0.4
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	1	0.4
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	1	0.4
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	2	0.39
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	5	0.39
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	5	0.39
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	7	0.39
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	7	0.39
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	1	0.39
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	1	0.39
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	1	0.39
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	10	0.39
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	10	0.39
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	10	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	1	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	1	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	1	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	3	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	3	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	3	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	6	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	6	0.39
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	6	0.39
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB1	9	0.39
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB2	9	0.39
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB3	9	0.39
(1,2200)	1:88:A:LEU:HD21	1:88:A:LEU:HA	4	0.39
(1,2200)	1:88:A:LEU:HD22	1:88:A:LEU:HA	4	0.39
(1,2200)	1:88:A:LEU:HD23	1:88:A:LEU:HA	4	0.39
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	9	0.39
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	9	0.39
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	9	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	4	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	4	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	4	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	4	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	4	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	4	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	5	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	5	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	5	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	5	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	5	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	5	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	8	0.39
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	8	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	8	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	8	0.39
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	8	0.39
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	9	0.39
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	9	0.39
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	9	0.39
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	3	0.39
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	3	0.39
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	3	0.39
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD11	7	0.39
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD12	7	0.39
(1,1036)	1:36:A:ILE:HA	1:36:A:ILE:HD13	7	0.39
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	6	0.39
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	6	0.39
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	6	0.39
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG11	6	0.39
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG12	6	0.39
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG13	6	0.39
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	2	0.39
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	2	0.39
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	2	0.39
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	9	0.39
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	9	0.39
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	9	0.39
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG11	4	0.39
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG12	4	0.39
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG13	4	0.39
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD11	4	0.39
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD12	4	0.39
(1,412)	1:15:A:ILE:HG21	1:15:A:ILE:HD13	4	0.39
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD11	4	0.39
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD12	4	0.39
(1,412)	1:15:A:ILE:HG22	1:15:A:ILE:HD13	4	0.39
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD11	4	0.39
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD12	4	0.39
(1,412)	1:15:A:ILE:HG23	1:15:A:ILE:HD13	4	0.39
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG21	4	0.39
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG22	4	0.39
(1,366)	1:15:A:ILE:HD11	1:15:A:ILE:HG23	4	0.39
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG21	4	0.39
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG22	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:15:A:ILE:HD12	1:15:A:ILE:HG23	4	0.39
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG21	4	0.39
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG22	4	0.39
(1,366)	1:15:A:ILE:HD13	1:15:A:ILE:HG23	4	0.39
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	8	0.39
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	8	0.39
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	8	0.39
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	3	0.38
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	3	0.38
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	8	0.38
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	8	0.38
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	8	0.38
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	7	0.38
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	7	0.38
(2,208)	1:40:A:TYR:HD1	1:41:A:GLU:H	1	0.38
(2,208)	1:40:A:TYR:HD2	1:41:A:GLU:H	1	0.38
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	9	0.38
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	9	0.38
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	9	0.38
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	4	0.38
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	4	0.38
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	4	0.38
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	7	0.38
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	7	0.38
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	7	0.38
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB2	1	0.38
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	1	0.38
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB2	3	0.38
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	3	0.38
(1,1975)	1:77:A:VAL:HG21	1:98:A:LEU:HD11	6	0.38
(1,1975)	1:77:A:VAL:HG21	1:98:A:LEU:HD12	6	0.38
(1,1975)	1:77:A:VAL:HG21	1:98:A:LEU:HD13	6	0.38
(1,1975)	1:77:A:VAL:HG22	1:98:A:LEU:HD11	6	0.38
(1,1975)	1:77:A:VAL:HG22	1:98:A:LEU:HD12	6	0.38
(1,1975)	1:77:A:VAL:HG22	1:98:A:LEU:HD13	6	0.38
(1,1975)	1:77:A:VAL:HG23	1:98:A:LEU:HD11	6	0.38
(1,1975)	1:77:A:VAL:HG23	1:98:A:LEU:HD12	6	0.38
(1,1975)	1:77:A:VAL:HG23	1:98:A:LEU:HD13	6	0.38
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	9	0.38
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	9	0.38
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	9	0.38
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	4	0.38
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	4	0.38
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	5	0.38
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	5	0.38
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	5	0.38
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD11	5	0.38
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD12	5	0.38
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD13	5	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG21	5	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG22	5	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG23	5	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG21	7	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG22	7	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG23	7	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG21	10	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG22	10	0.38
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG23	10	0.38
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD11	9	0.38
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD12	9	0.38
(1,1209)	1:40:A:TYR:HE1	1:95:A:LEU:HD13	9	0.38
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD11	9	0.38
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD12	9	0.38
(1,1209)	1:40:A:TYR:HE2	1:95:A:LEU:HD13	9	0.38
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	10	0.38
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	10	0.38
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	10	0.38
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG11	1	0.38
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG12	1	0.38
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG13	1	0.38
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	6	0.38
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	6	0.38
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	6	0.38
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE1	4	0.37
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE2	4	0.37
(2,325)	1:69:A:ILE:HG21	1:71:A:SER:HA	8	0.37
(2,325)	1:69:A:ILE:HG22	1:71:A:SER:HA	8	0.37
(2,325)	1:69:A:ILE:HG23	1:71:A:SER:HA	8	0.37
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	2	0.37
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	2	0.37
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	3	0.37
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	3	0.37
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE1	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE2	1	0.37
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE1	7	0.37
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE2	7	0.37
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	1	0.37
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	1	0.37
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	1	0.37
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	1	0.37
(2,34)	1:3:A:LYS:HE2	1:5:A:VAL:HB	10	0.37
(2,34)	1:3:A:LYS:HE3	1:5:A:VAL:HB	10	0.37
(1,2545)	1:27:A:ALA:HB1	1:27:A:ALA:HA	5	0.37
(1,2545)	1:27:A:ALA:HB2	1:27:A:ALA:HA	5	0.37
(1,2545)	1:27:A:ALA:HB3	1:27:A:ALA:HA	5	0.37
(1,2197)	1:88:A:LEU:HD11	1:89:A:GLY:H	8	0.37
(1,2197)	1:88:A:LEU:HD12	1:89:A:GLY:H	8	0.37
(1,2197)	1:88:A:LEU:HD13	1:89:A:GLY:H	8	0.37
(1,2197)	1:88:A:LEU:HD21	1:89:A:GLY:H	8	0.37
(1,2197)	1:88:A:LEU:HD22	1:89:A:GLY:H	8	0.37
(1,2197)	1:88:A:LEU:HD23	1:89:A:GLY:H	8	0.37
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE1	3	0.37
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE2	3	0.37
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE1	3	0.37
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE2	3	0.37
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE1	3	0.37
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE2	3	0.37
(1,1960)	1:77:A:VAL:HG11	1:102:A:TYR:HD1	9	0.37
(1,1960)	1:77:A:VAL:HG11	1:102:A:TYR:HD2	9	0.37
(1,1960)	1:77:A:VAL:HG12	1:102:A:TYR:HD1	9	0.37
(1,1960)	1:77:A:VAL:HG12	1:102:A:TYR:HD2	9	0.37
(1,1960)	1:77:A:VAL:HG13	1:102:A:TYR:HD1	9	0.37
(1,1960)	1:77:A:VAL:HG13	1:102:A:TYR:HD2	9	0.37
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	3	0.37
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	3	0.37
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	3	0.37
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	3	0.37
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	3	0.37
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	3	0.37
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	7	0.37
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	7	0.37
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	7	0.37
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	7	0.37
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	7	0.37
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	7	0.37
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	7	0.37
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	7	0.37
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG21	1	0.37
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG22	1	0.37
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG23	1	0.37
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	3	0.37
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	3	0.37
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB1	9	0.37
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB2	9	0.37
(1,936)	1:27:A:ALA:H	1:27:A:ALA:HB3	9	0.37
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	5	0.37
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	5	0.37
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	5	0.37
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	8	0.37
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	8	0.37
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	8	0.37
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	4	0.37
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	4	0.37
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	4	0.37
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	4	0.37
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	4	0.37
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	4	0.37
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG11	3	0.37
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG12	3	0.37
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG13	3	0.37
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	10	0.37
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	10	0.37
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	10	0.37
(1,431)	1:15:A:ILE:HG21	1:81:A:GLY:HA2	1	0.37
(1,431)	1:15:A:ILE:HG22	1:81:A:GLY:HA2	1	0.37
(1,431)	1:15:A:ILE:HG23	1:81:A:GLY:HA2	1	0.37
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	6	0.37
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	6	0.37
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	6	0.37
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	7	0.36
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	7	0.36
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	7	0.36
(1,2548)	1:27:A:ALA:HB1	1:29:A:TRP:H	3	0.36
(1,2548)	1:27:A:ALA:HB2	1:29:A:TRP:H	3	0.36
(1,2548)	1:27:A:ALA:HB3	1:29:A:TRP:H	3	0.36
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	1	0.36
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	1	0.36
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB1	10	0.36
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB2	10	0.36
(1,2238)	1:91:A:ASN:HB2	1:94:A:ALA:HB3	10	0.36
(1,2197)	1:88:A:LEU:HD11	1:89:A:GLY:H	7	0.36
(1,2197)	1:88:A:LEU:HD12	1:89:A:GLY:H	7	0.36
(1,2197)	1:88:A:LEU:HD13	1:89:A:GLY:H	7	0.36
(1,2197)	1:88:A:LEU:HD21	1:89:A:GLY:H	7	0.36
(1,2197)	1:88:A:LEU:HD22	1:89:A:GLY:H	7	0.36
(1,2197)	1:88:A:LEU:HD23	1:89:A:GLY:H	7	0.36
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	5	0.36
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	5	0.36
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	5	0.36
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	7	0.36
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	7	0.36
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	7	0.36
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	2	0.36
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	2	0.36
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	2	0.36
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD11	6	0.36
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD12	6	0.36
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD13	6	0.36
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG21	4	0.36
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG22	4	0.36
(1,1458)	1:51:A:VAL:H	1:51:A:VAL:HG23	4	0.36
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD1	4	0.36
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD2	4	0.36
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD1	5	0.36
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD2	5	0.36
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	6	0.36
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	6	0.36
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	8	0.36
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	8	0.36
(1,712)	1:23:A:VAL:HG11	1:25:A:PHE:HZ	7	0.36
(1,712)	1:23:A:VAL:HG12	1:25:A:PHE:HZ	7	0.36
(1,712)	1:23:A:VAL:HG13	1:25:A:PHE:HZ	7	0.36
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	5	0.36
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	5	0.36
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	5	0.36
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	7	0.36
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	7	0.36
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE1	9	0.35
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE2	9	0.35
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	5	0.35
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	5	0.35
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	5	0.35
(2,234)	1:44:A:SER:HG	1:52:A:PHE:HD1	9	0.35
(2,234)	1:44:A:SER:HG	1:52:A:PHE:HD2	9	0.35
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE1	1	0.35
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE2	1	0.35
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE3	1	0.35
(1,2549)	1:27:A:ALA:HB1	1:30:A:CYS:HB3	5	0.35
(1,2549)	1:27:A:ALA:HB2	1:30:A:CYS:HB3	5	0.35
(1,2549)	1:27:A:ALA:HB3	1:30:A:CYS:HB3	5	0.35
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	3	0.35
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	3	0.35
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	3	0.35
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB2	9	0.35
(1,2351)	1:97:A:GLN:HE21	1:97:A:GLN:HB3	9	0.35
(1,2271)	1:93:A:SER:HB2	1:97:A:GLN:HE22	6	0.35
(1,2271)	1:93:A:SER:HB3	1:97:A:GLN:HE22	6	0.35
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB1	2	0.35
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB2	2	0.35
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB3	2	0.35
(1,2172)	1:87:A:LEU:HD11	1:91:A:ASN:HB2	10	0.35
(1,2172)	1:87:A:LEU:HD12	1:91:A:ASN:HB2	10	0.35
(1,2172)	1:87:A:LEU:HD13	1:91:A:ASN:HB2	10	0.35
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB1	3	0.35
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB2	3	0.35
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB3	3	0.35
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	9	0.35
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	9	0.35
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	9	0.35
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	9	0.35
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	9	0.35
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	9	0.35
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	9	0.35
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	9	0.35
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	9	0.35
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	2	0.35
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	2	0.35
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD1	10	0.35
(1,1270)	1:43:A:CYS:HB2	1:47:A:TYR:HD2	10	0.35
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	1	0.35
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	1	0.35
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	1	0.35
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	1	0.35
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	1	0.35
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	2	0.35
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	2	0.35
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	10	0.35
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	10	0.35
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	10	0.35
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	10	0.35
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	10	0.35
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	10	0.35
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	3	0.35
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	3	0.35
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	3	0.35
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE1	2	0.34
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE2	2	0.34
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD11	6	0.34
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD12	6	0.34
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD13	6	0.34
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	4	0.34
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	4	0.34
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	4	0.34
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE2	2	0.34
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE3	2	0.34
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	2	0.34
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	2	0.34
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	4	0.34
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	4	0.34
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	4	0.34
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	4	0.34
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	4	0.34
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	4	0.34
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	4	0.34
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	4	0.34
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	4	0.34
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	1	0.34
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	1	0.34
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	1	0.34
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	1	0.34
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	1	0.34
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	10	0.34
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	10	0.34
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	10	0.34
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	10	0.34
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	10	0.34
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	10	0.34
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	6	0.34
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	6	0.34
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	6	0.34
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD1	3	0.34
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD2	3	0.34
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD1	3	0.34
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD2	3	0.34
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD1	3	0.34
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD2	3	0.34
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	7	0.34
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	7	0.34
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	8	0.34
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	8	0.34
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	8	0.34
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	8	0.34
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	8	0.34
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	8	0.34
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG21	8	0.34
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG22	8	0.34
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG23	8	0.34
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG21	8	0.34
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG22	8	0.34
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG23	8	0.34
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG21	8	0.34
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG22	8	0.34
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG23	8	0.34
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	3	0.34
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	3	0.34
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	3	0.34
(1,747)	1:23:A:VAL:HG21	1:53:A:ILE:HG12	8	0.34
(1,747)	1:23:A:VAL:HG22	1:53:A:ILE:HG12	8	0.34
(1,747)	1:23:A:VAL:HG23	1:53:A:ILE:HG12	8	0.34
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	9	0.33
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	9	0.33
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	3	0.33
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	3	0.33
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE1	5	0.33
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE2	5	0.33
(2,209)	1:40:A:TYR:HD1	1:43:A:CYS:H	1	0.33
(2,209)	1:40:A:TYR:HD2	1:43:A:CYS:H	1	0.33
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	10	0.33
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	10	0.33
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG21	7	0.33
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG22	7	0.33
(1,2429)	1:99:A:ILE:H	1:99:A:ILE:HG23	7	0.33
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	5	0.33
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	5	0.33
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	5	0.33
(1,2123)	1:84:A:VAL:HG11	1:85:A:ASP:H	10	0.33
(1,2123)	1:84:A:VAL:HG12	1:85:A:ASP:H	10	0.33
(1,2123)	1:84:A:VAL:HG13	1:85:A:ASP:H	10	0.33
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	1	0.33
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	1	0.33
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	1	0.33
(1,1959)	1:77:A:VAL:HG11	1:102:A:TYR:HB2	9	0.33
(1,1959)	1:77:A:VAL:HG12	1:102:A:TYR:HB2	9	0.33
(1,1959)	1:77:A:VAL:HG13	1:102:A:TYR:HB2	9	0.33
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	4	0.33
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	4	0.33
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	4	0.33
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	7	0.33
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	7	0.33
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	7	0.33
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	5	0.33
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	5	0.33
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	5	0.33
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	6	0.33
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	6	0.33
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	6	0.33
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	7	0.32
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	7	0.32
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	8	0.32
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	8	0.32
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	7	0.32
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE2	9	0.32
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE3	9	0.32
(1,2197)	1:88:A:LEU:HD11	1:89:A:GLY:H	3	0.32
(1,2197)	1:88:A:LEU:HD12	1:89:A:GLY:H	3	0.32
(1,2197)	1:88:A:LEU:HD13	1:89:A:GLY:H	3	0.32
(1,2197)	1:88:A:LEU:HD21	1:89:A:GLY:H	3	0.32
(1,2197)	1:88:A:LEU:HD22	1:89:A:GLY:H	3	0.32
(1,2197)	1:88:A:LEU:HD23	1:89:A:GLY:H	3	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	4	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	4	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	4	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	7	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	7	0.32
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	7	0.32
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG21	6	0.32
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG22	6	0.32
(1,1916)	1:76:A:LYS:HD2	1:86:A:THR:HG23	6	0.32
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG21	6	0.32
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG22	6	0.32
(1,1916)	1:76:A:LYS:HD3	1:86:A:THR:HG23	6	0.32
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	6	0.32
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	6	0.32
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	6	0.32
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	6	0.32
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	6	0.32
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	6	0.32
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	6	0.32
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	6	0.32
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	9	0.32
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	9	0.32
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	9	0.32
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	9	0.32
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	9	0.32
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	9	0.32
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	2	0.32
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	2	0.32
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB1	6	0.32
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB2	6	0.32
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB3	6	0.32
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG21	10	0.32
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG22	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG23	10	0.32
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG21	10	0.32
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG22	10	0.32
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG23	10	0.32
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG21	10	0.32
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG22	10	0.32
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG23	10	0.32
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	5	0.32
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	5	0.32
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	5	0.32
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	5	0.32
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	5	0.32
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	5	0.32
(1,633)	1:22:A:ILE:HA	1:22:A:ILE:HD11	8	0.32
(1,633)	1:22:A:ILE:HA	1:22:A:ILE:HD12	8	0.32
(1,633)	1:22:A:ILE:HA	1:22:A:ILE:HD13	8	0.32
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	3	0.32
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	3	0.32
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	5	0.32
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	5	0.32
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	5	0.32
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE1	10	0.31
(2,296)	1:67:A:GLU:HB3	1:78:A:TYR:HE2	10	0.31
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	8	0.31
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	8	0.31
(1,2549)	1:27:A:ALA:HB1	1:30:A:CYS:HB3	2	0.31
(1,2549)	1:27:A:ALA:HB2	1:30:A:CYS:HB3	2	0.31
(1,2549)	1:27:A:ALA:HB3	1:30:A:CYS:HB3	2	0.31
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	5	0.31
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	5	0.31
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	5	0.31
(1,2542)	1:26:A:PHE:HE1	1:55:A:VAL:HA	10	0.31
(1,2542)	1:26:A:PHE:HE2	1:55:A:VAL:HA	10	0.31
(1,2314)	1:95:A:LEU:HG	1:99:A:ILE:HG21	7	0.31
(1,2314)	1:95:A:LEU:HG	1:99:A:ILE:HG22	7	0.31
(1,2314)	1:95:A:LEU:HG	1:99:A:ILE:HG23	7	0.31
(1,2270)	1:93:A:SER:HB2	1:97:A:GLN:HE21	4	0.31
(1,2270)	1:93:A:SER:HB3	1:97:A:GLN:HE21	4	0.31
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD21	2	0.31
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD22	2	0.31
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD23	2	0.31
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD21	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD22	2	0.31
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD23	2	0.31
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD21	2	0.31
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD22	2	0.31
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD23	2	0.31
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	9	0.31
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	9	0.31
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	9	0.31
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	9	0.31
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	9	0.31
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	9	0.31
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	9	0.31
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	9	0.31
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	9	0.31
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	3	0.31
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	3	0.31
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	5	0.31
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	5	0.31
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	5	0.31
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	5	0.31
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	5	0.31
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	5	0.31
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	5	0.31
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	5	0.31
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	5	0.31
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD11	4	0.31
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD12	4	0.31
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD13	4	0.31
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	7	0.31
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	7	0.31
(1,1376)	1:47:A:TYR:HD1	1:99:A:ILE:HG12	8	0.31
(1,1376)	1:47:A:TYR:HD2	1:99:A:ILE:HG12	8	0.31
(1,1336)	1:46:A:THR:HG21	1:47:A:TYR:H	5	0.31
(1,1336)	1:46:A:THR:HG22	1:47:A:TYR:H	5	0.31
(1,1336)	1:46:A:THR:HG23	1:47:A:TYR:H	5	0.31
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	5	0.31
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	5	0.31
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	5	0.31
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	4	0.31
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	4	0.31
(1,798)	1:25:A:PHE:HA	1:25:A:PHE:HD1	2	0.31
(1,798)	1:25:A:PHE:HA	1:25:A:PHE:HD2	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	2	0.31
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	2	0.31
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	2	0.31
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG11	2	0.31
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG12	2	0.31
(1,692)	1:22:A:ILE:H	1:51:A:VAL:HG13	2	0.31
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	7	0.31
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	7	0.31
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	7	0.31
(1,382)	1:15:A:ILE:HD11	1:23:A:VAL:HG21	1	0.31
(1,382)	1:15:A:ILE:HD11	1:23:A:VAL:HG22	1	0.31
(1,382)	1:15:A:ILE:HD11	1:23:A:VAL:HG23	1	0.31
(1,382)	1:15:A:ILE:HD12	1:23:A:VAL:HG21	1	0.31
(1,382)	1:15:A:ILE:HD12	1:23:A:VAL:HG22	1	0.31
(1,382)	1:15:A:ILE:HD12	1:23:A:VAL:HG23	1	0.31
(1,382)	1:15:A:ILE:HD13	1:23:A:VAL:HG21	1	0.31
(1,382)	1:15:A:ILE:HD13	1:23:A:VAL:HG22	1	0.31
(1,382)	1:15:A:ILE:HD13	1:23:A:VAL:HG23	1	0.31
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG11	3	0.31
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG12	3	0.31
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG13	3	0.31
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG11	3	0.31
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG12	3	0.31
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG13	3	0.31
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	7	0.31
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	7	0.31
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD1	8	0.31
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD2	8	0.31
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	3	0.31
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	3	0.31
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	3	0.31
(1,20)	1:2:A:VAL:HG21	1:40:A:TYR:HD1	10	0.31
(1,20)	1:2:A:VAL:HG21	1:40:A:TYR:HD2	10	0.31
(1,20)	1:2:A:VAL:HG22	1:40:A:TYR:HD1	10	0.31
(1,20)	1:2:A:VAL:HG22	1:40:A:TYR:HD2	10	0.31
(1,20)	1:2:A:VAL:HG23	1:40:A:TYR:HD1	10	0.31
(1,20)	1:2:A:VAL:HG23	1:40:A:TYR:HD2	10	0.31
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	9	0.3
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	9	0.3
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	9	0.3
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	9	0.3
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	9	0.3
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	9	0.3
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	9	0.3
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	9	0.3
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	5	0.3
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	5	0.3
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE1	9	0.3
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE2	9	0.3
(2,245)	1:47:A:TYR:HB3	1:50:A:MET:HE3	9	0.3
(2,151)	1:27:A:ALA:HB1	1:58:A:ASP:HB2	1	0.3
(2,151)	1:27:A:ALA:HB2	1:58:A:ASP:HB2	1	0.3
(2,151)	1:27:A:ALA:HB3	1:58:A:ASP:HB2	1	0.3
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE1	7	0.3
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE2	7	0.3
(2,131)	1:26:A:PHE:HA	1:72:A:MET:HE3	7	0.3
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	8	0.3
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	8	0.3
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	6	0.3
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	6	0.3
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	8	0.3
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	8	0.3
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	8	0.3
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	8	0.3
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	8	0.3
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	8	0.3
(1,2052)	1:79:A:LYS:HD2	1:80:A:ASN:H	5	0.3
(1,2052)	1:79:A:LYS:HD3	1:80:A:ASN:H	5	0.3
(1,2052)	1:79:A:LYS:HD2	1:80:A:ASN:H	7	0.3
(1,2052)	1:79:A:LYS:HD3	1:80:A:ASN:H	7	0.3
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	8	0.3
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	8	0.3
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	8	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	1	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	1	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	5	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	5	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	8	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	8	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	10	0.3
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	10	0.3
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD21	6	0.3
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD22	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	1:75:A:PHE:HB2	1:87:A:LEU:HD23	6	0.3
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	4	0.3
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	4	0.3
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	4	0.3
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	10	0.3
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	10	0.3
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	10	0.3
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	10	0.3
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	10	0.3
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	10	0.3
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	10	0.3
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	10	0.3
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	10	0.3
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	8	0.3
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	8	0.3
(1,1054)	1:36:A:ILE:HD11	1:91:A:ASN:H	2	0.3
(1,1054)	1:36:A:ILE:HD12	1:91:A:ASN:H	2	0.3
(1,1054)	1:36:A:ILE:HD13	1:91:A:ASN:H	2	0.3
(1,798)	1:25:A:PHE:HA	1:25:A:PHE:HD1	7	0.3
(1,798)	1:25:A:PHE:HA	1:25:A:PHE:HD2	7	0.3
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	6	0.3
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	6	0.3
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	6	0.3
(1,585)	1:20:A:LEU:HG	1:21:A:VAL:H	5	0.3
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG21	2	0.3
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG22	2	0.3
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG23	2	0.3
(1,431)	1:15:A:ILE:HG21	1:81:A:GLY:HA2	2	0.3
(1,431)	1:15:A:ILE:HG22	1:81:A:GLY:HA2	2	0.3
(1,431)	1:15:A:ILE:HG23	1:81:A:GLY:HA2	2	0.3
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	5	0.3
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	5	0.3
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	8	0.3
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	8	0.3
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	6	0.29
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	6	0.29
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	6	0.29
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	6	0.29
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	6	0.29
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	6	0.29
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	6	0.29
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	6	0.29
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	4	0.29
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	4	0.29
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	2	0.29
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	2	0.29
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	2	0.29
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	7	0.29
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	7	0.29
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	5	0.29
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	5	0.29
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	5	0.29
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	5	0.29
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	5	0.29
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	5	0.29
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	5	0.29
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	5	0.29
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	10	0.29
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	10	0.29
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	10	0.29
(1,1960)	1:77:A:VAL:HG11	1:102:A:TYR:HD1	1	0.29
(1,1960)	1:77:A:VAL:HG11	1:102:A:TYR:HD2	1	0.29
(1,1960)	1:77:A:VAL:HG12	1:102:A:TYR:HD1	1	0.29
(1,1960)	1:77:A:VAL:HG12	1:102:A:TYR:HD2	1	0.29
(1,1960)	1:77:A:VAL:HG13	1:102:A:TYR:HD1	1	0.29
(1,1960)	1:77:A:VAL:HG13	1:102:A:TYR:HD2	1	0.29
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	8	0.29
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	8	0.29
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	8	0.29
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	8	0.29
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	8	0.29
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	8	0.29
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	8	0.29
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	8	0.29
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	8	0.29
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG2	4	0.29
(1,1896)	1:76:A:LYS:HA	1:76:A:LYS:HG3	4	0.29
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	8	0.29
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	8	0.29
(1,1376)	1:47:A:TYR:HD1	1:99:A:ILE:HG12	4	0.29
(1,1376)	1:47:A:TYR:HD2	1:99:A:ILE:HG12	4	0.29
(1,1376)	1:47:A:TYR:HD1	1:99:A:ILE:HG12	6	0.29
(1,1376)	1:47:A:TYR:HD2	1:99:A:ILE:HG12	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD1	9	0.29
(1,1263)	1:43:A:CYS:HB3	1:47:A:TYR:HD2	9	0.29
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	5	0.29
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	5	0.29
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	5	0.29
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	5	0.29
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	5	0.29
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	5	0.29
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	1	0.29
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	1	0.29
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	1	0.29
(1,233)	1:11:A:PHE:HE1	1:67:A:GLU:HG2	8	0.29
(1,233)	1:11:A:PHE:HE1	1:67:A:GLU:HG3	8	0.29
(1,233)	1:11:A:PHE:HE2	1:67:A:GLU:HG2	8	0.29
(1,233)	1:11:A:PHE:HE2	1:67:A:GLU:HG3	8	0.29
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	6	0.29
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	6	0.29
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	4	0.29
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	4	0.29
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	4	0.29
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	6	0.29
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	6	0.29
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	6	0.29
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE1	9	0.28
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE2	9	0.28
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	10	0.28
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	10	0.28
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE1	3	0.28
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE2	3	0.28
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	2	0.28
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	2	0.28
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	4	0.28
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	4	0.28
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	4	0.28
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	9	0.28
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	9	0.28
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	9	0.28
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	9	0.28
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	9	0.28
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	9	0.28
(1,2172)	1:87:A:LEU:HD11	1:91:A:ASN:HB2	3	0.28
(1,2172)	1:87:A:LEU:HD12	1:91:A:ASN:HB2	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2172)	1:87:A:LEU:HD13	1:91:A:ASN:HB2	3	0.28
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	4	0.28
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	4	0.28
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	4	0.28
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD21	10	0.28
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD22	10	0.28
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD23	10	0.28
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD21	10	0.28
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD22	10	0.28
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD23	10	0.28
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD21	10	0.28
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD22	10	0.28
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD23	10	0.28
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	7	0.28
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	7	0.28
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	7	0.28
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD11	1	0.28
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD12	1	0.28
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD13	1	0.28
(1,1685)	1:66:A:LYS:HG2	1:67:A:GLU:H	7	0.28
(1,1685)	1:66:A:LYS:HG3	1:67:A:GLU:H	7	0.28
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	8	0.28
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	8	0.28
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	8	0.28
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	10	0.28
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	10	0.28
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	10	0.28
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	4	0.28
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	4	0.28
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	5	0.28
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	5	0.28
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	6	0.28
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	6	0.28
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	4	0.28
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	4	0.28
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	4	0.28
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD1	10	0.28
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD2	10	0.28
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD1	10	0.28
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD2	10	0.28
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD1	10	0.28
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD2	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	4	0.28
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	4	0.28
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	4	0.28
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	4	0.28
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	4	0.28
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	4	0.28
(1,746)	1:23:A:VAL:HG21	1:53:A:ILE:HG13	1	0.28
(1,746)	1:23:A:VAL:HG22	1:53:A:ILE:HG13	1	0.28
(1,746)	1:23:A:VAL:HG23	1:53:A:ILE:HG13	1	0.28
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	10	0.28
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	10	0.28
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	10	0.28
(1,723)	1:23:A:VAL:HG11	1:55:A:VAL:HG21	1	0.28
(1,723)	1:23:A:VAL:HG11	1:55:A:VAL:HG22	1	0.28
(1,723)	1:23:A:VAL:HG11	1:55:A:VAL:HG23	1	0.28
(1,723)	1:23:A:VAL:HG12	1:55:A:VAL:HG21	1	0.28
(1,723)	1:23:A:VAL:HG12	1:55:A:VAL:HG22	1	0.28
(1,723)	1:23:A:VAL:HG12	1:55:A:VAL:HG23	1	0.28
(1,723)	1:23:A:VAL:HG13	1:55:A:VAL:HG21	1	0.28
(1,723)	1:23:A:VAL:HG13	1:55:A:VAL:HG22	1	0.28
(1,723)	1:23:A:VAL:HG13	1:55:A:VAL:HG23	1	0.28
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG11	7	0.28
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG12	7	0.28
(1,575)	1:20:A:LEU:HD11	1:77:A:VAL:HG13	7	0.28
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG11	7	0.28
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG12	7	0.28
(1,575)	1:20:A:LEU:HD12	1:77:A:VAL:HG13	7	0.28
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG11	7	0.28
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG12	7	0.28
(1,575)	1:20:A:LEU:HD13	1:77:A:VAL:HG13	7	0.28
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG11	6	0.28
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG12	6	0.28
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG13	6	0.28
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG11	6	0.28
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG12	6	0.28
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG13	6	0.28
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	1	0.28
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	1	0.28
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	4	0.28
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	4	0.28
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	10	0.28
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG21	9	0.28
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG22	9	0.28
(1,30)	1:2:A:VAL:H	1:2:A:VAL:HG23	9	0.28
(2,284)	1:57:A:VAL:HG11	1:61:A:SER:HA	6	0.27
(2,284)	1:57:A:VAL:HG12	1:61:A:SER:HA	6	0.27
(2,284)	1:57:A:VAL:HG13	1:61:A:SER:HA	6	0.27
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	8	0.27
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	8	0.27
(2,9)	1:1:A:SER:HB2	1:2:A:VAL:HA	1	0.27
(2,9)	1:1:A:SER:HB3	1:2:A:VAL:HA	1	0.27
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	10	0.27
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	10	0.27
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	10	0.27
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	10	0.27
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	10	0.27
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	10	0.27
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	10	0.27
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	10	0.27
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	10	0.27
(1,2271)	1:93:A:SER:HB2	1:97:A:GLN:HE22	2	0.27
(1,2271)	1:93:A:SER:HB3	1:97:A:GLN:HE22	2	0.27
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	3	0.27
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	3	0.27
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	3	0.27
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD21	4	0.27
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD22	4	0.27
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD23	4	0.27
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD21	4	0.27
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD22	4	0.27
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD23	4	0.27
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD21	4	0.27
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD22	4	0.27
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD23	4	0.27
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	9	0.27
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	9	0.27
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	9	0.27
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	9	0.27
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	9	0.27
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	9	0.27
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	9	0.27
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	9	0.27
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	1	0.27
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	1	0.27
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	1	0.27
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	10	0.27
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	10	0.27
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	10	0.27
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	6	0.27
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	6	0.27
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	6	0.27
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	6	0.27
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	6	0.27
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	6	0.27
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	6	0.27
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	6	0.27
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	6	0.27
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	1	0.27
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	1	0.27
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG21	5	0.27
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG22	5	0.27
(1,1392)	1:47:A:TYR:HE1	1:99:A:ILE:HG23	5	0.27
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG21	5	0.27
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG22	5	0.27
(1,1392)	1:47:A:TYR:HE2	1:99:A:ILE:HG23	5	0.27
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	7	0.27
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	7	0.27
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	7	0.27
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	7	0.27
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	7	0.27
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	7	0.27
(1,844)	1:25:A:PHE:HE1	1:76:A:LYS:HE3	2	0.27
(1,844)	1:25:A:PHE:HE2	1:76:A:LYS:HE3	2	0.27
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	2	0.27
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	2	0.27
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	2	0.27
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	10	0.27
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	10	0.27
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	10	0.27
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	10	0.27
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	10	0.27
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	10	0.27
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	4	0.27
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	4	0.27
(1,573)	1:20:A:LEU:HB2	1:79:A:LYS:HA	5	0.27
(1,573)	1:20:A:LEU:HB3	1:79:A:LYS:HA	5	0.27
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG2	8	0.27
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG3	8	0.27
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	2	0.27
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	2	0.27
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD1	9	0.27
(1,154)	1:8:A:GLN:HE22	1:11:A:PHE:HD2	9	0.27
(1,112)	1:6:A:THR:H	1:6:A:THR:HG21	3	0.27
(1,112)	1:6:A:THR:H	1:6:A:THR:HG22	3	0.27
(1,112)	1:6:A:THR:H	1:6:A:THR:HG23	3	0.27
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB1	10	0.26
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB2	10	0.26
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB3	10	0.26
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	2	0.26
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	2	0.26
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	5	0.26
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	5	0.26
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	4	0.26
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	4	0.26
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	4	0.26
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	6	0.26
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	6	0.26
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	6	0.26
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	7	0.26
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	7	0.26
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	7	0.26
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	4	0.26
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	4	0.26
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	4	0.26
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	6	0.26
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	6	0.26
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	6	0.26
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	7	0.26
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	7	0.26
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	7	0.26
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB1	4	0.26
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB2	4	0.26
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB3	4	0.26
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB1	8	0.26
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB2	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2244)	1:91:A:ASN:HD21	1:94:A:ALA:HB3	8	0.26
(1,2172)	1:87:A:LEU:HD11	1:91:A:ASN:HB2	5	0.26
(1,2172)	1:87:A:LEU:HD12	1:91:A:ASN:HB2	5	0.26
(1,2172)	1:87:A:LEU:HD13	1:91:A:ASN:HB2	5	0.26
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	1	0.26
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	1	0.26
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	1	0.26
(1,1959)	1:77:A:VAL:HG11	1:102:A:TYR:HB2	10	0.26
(1,1959)	1:77:A:VAL:HG12	1:102:A:TYR:HB2	10	0.26
(1,1959)	1:77:A:VAL:HG13	1:102:A:TYR:HB2	10	0.26
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	10	0.26
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	10	0.26
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	10	0.26
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	10	0.26
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	10	0.26
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	10	0.26
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	10	0.26
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	10	0.26
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	10	0.26
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	7	0.26
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	7	0.26
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	7	0.26
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	8	0.26
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	8	0.26
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	8	0.26
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	6	0.26
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	6	0.26
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	6	0.26
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG21	10	0.26
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG22	10	0.26
(1,1778)	1:70:A:THR:H	1:70:A:THR:HG23	10	0.26
(1,1488)	1:52:A:PHE:HZ	1:99:A:ILE:HG12	7	0.26
(1,1376)	1:47:A:TYR:HD1	1:99:A:ILE:HG12	7	0.26
(1,1376)	1:47:A:TYR:HD2	1:99:A:ILE:HG12	7	0.26
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	10	0.26
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	10	0.26
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG21	2	0.26
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG22	2	0.26
(1,752)	1:23:A:VAL:HG21	1:55:A:VAL:HG23	2	0.26
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG21	2	0.26
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG22	2	0.26
(1,752)	1:23:A:VAL:HG22	1:55:A:VAL:HG23	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG21	2	0.26
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG22	2	0.26
(1,752)	1:23:A:VAL:HG23	1:55:A:VAL:HG23	2	0.26
(1,665)	1:22:A:ILE:HG21	1:50:A:MET:HB3	8	0.26
(1,665)	1:22:A:ILE:HG22	1:50:A:MET:HB3	8	0.26
(1,665)	1:22:A:ILE:HG23	1:50:A:MET:HB3	8	0.26
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	9	0.26
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG11	1	0.26
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG12	1	0.26
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG13	1	0.26
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD1	1	0.26
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD2	1	0.26
(1,112)	1:6:A:THR:H	1:6:A:THR:HG21	9	0.26
(1,112)	1:6:A:THR:H	1:6:A:THR:HG22	9	0.26
(1,112)	1:6:A:THR:H	1:6:A:THR:HG23	9	0.26
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	8	0.25
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	8	0.25
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	8	0.25
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE2	1	0.25
(2,230)	1:44:A:SER:HG	1:45:A:LYS:HE3	1	0.25
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	6	0.25
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	6	0.25
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	6	0.25
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	6	0.25
(1,2547)	1:27:A:ALA:HB1	1:29:A:TRP:HE1	7	0.25
(1,2547)	1:27:A:ALA:HB2	1:29:A:TRP:HE1	7	0.25
(1,2547)	1:27:A:ALA:HB3	1:29:A:TRP:HE1	7	0.25
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	7	0.25
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	7	0.25
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	7	0.25
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	9	0.25
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	9	0.25
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	9	0.25
(1,2388)	1:98:A:LEU:HD21	1:99:A:ILE:HA	3	0.25
(1,2388)	1:98:A:LEU:HD22	1:99:A:ILE:HA	3	0.25
(1,2388)	1:98:A:LEU:HD23	1:99:A:ILE:HA	3	0.25
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	3	0.25
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	3	0.25
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	3	0.25
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	3	0.25
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	3	0.25
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	8	0.25
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	8	0.25
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	8	0.25
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD1	5	0.25
(1,1980)	1:77:A:VAL:HG21	1:102:A:TYR:HD2	5	0.25
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD1	5	0.25
(1,1980)	1:77:A:VAL:HG22	1:102:A:TYR:HD2	5	0.25
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD1	5	0.25
(1,1980)	1:77:A:VAL:HG23	1:102:A:TYR:HD2	5	0.25
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	5	0.25
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	5	0.25
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	5	0.25
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	5	0.25
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	5	0.25
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	5	0.25
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	5	0.25
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	5	0.25
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	5	0.25
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	7	0.25
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	7	0.25
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	7	0.25
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	7	0.25
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	7	0.25
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	7	0.25
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	7	0.25
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	7	0.25
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	7	0.25
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	6	0.25
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	6	0.25
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	6	0.25
(1,1550)	1:57:A:VAL:HG21	1:58:A:ASP:H	1	0.25
(1,1550)	1:57:A:VAL:HG22	1:58:A:ASP:H	1	0.25
(1,1550)	1:57:A:VAL:HG23	1:58:A:ASP:H	1	0.25
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	10	0.25
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	10	0.25
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	10	0.25
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	10	0.25
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	10	0.25
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	10	0.25
(1,1225)	1:41:A:GLU:HG2	1:42:A:GLU:H	1	0.25
(1,1225)	1:41:A:GLU:HG3	1:42:A:GLU:H	1	0.25
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	1	0.25
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	1	0.25
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB1	1	0.25
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB2	1	0.25
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB3	1	0.25
(1,826)	1:25:A:PHE:HD1	1:25:A:PHE:H	6	0.25
(1,826)	1:25:A:PHE:HD2	1:25:A:PHE:H	6	0.25
(1,826)	1:25:A:PHE:HD1	1:25:A:PHE:H	8	0.25
(1,826)	1:25:A:PHE:HD2	1:25:A:PHE:H	8	0.25
(1,826)	1:25:A:PHE:HD1	1:25:A:PHE:H	9	0.25
(1,826)	1:25:A:PHE:HD2	1:25:A:PHE:H	9	0.25
(1,749)	1:23:A:VAL:HG21	1:54:A:LYS:HA	8	0.25
(1,749)	1:23:A:VAL:HG22	1:54:A:LYS:HA	8	0.25
(1,749)	1:23:A:VAL:HG23	1:54:A:LYS:HA	8	0.25
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	3	0.25
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	3	0.25
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	3	0.25
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	3	0.25
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	3	0.25
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	3	0.25
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG21	10	0.25
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG22	10	0.25
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG23	10	0.25
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD11	1	0.25
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD12	1	0.25
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD13	1	0.25
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG11	4	0.25
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG12	4	0.25
(1,97)	1:5:A:VAL:H	1:5:A:VAL:HG13	4	0.25
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD11	7	0.24
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD12	7	0.24
(2,304)	1:68:A:ASN:HD22	1:69:A:ILE:HD13	7	0.24
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE1	1	0.24
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE2	1	0.24
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	6	0.24
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	6	0.24
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	8	0.24
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	8	0.24
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE1	10	0.24
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE2	10	0.24
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE3	10	0.24
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	9	0.24
(2,34)	1:3:A:LYS:HE2	1:5:A:VAL:HB	9	0.24
(2,34)	1:3:A:LYS:HE3	1:5:A:VAL:HB	9	0.24
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	6	0.24
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	6	0.24
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	6	0.24
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	1	0.24
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	1	0.24
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	1	0.24
(1,2304)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	2	0.24
(1,2304)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	2	0.24
(1,2304)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	2	0.24
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	1	0.24
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	1	0.24
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	1	0.24
(1,2303)	1:95:A:LEU:HD11	1:95:A:LEU:HB2	2	0.24
(1,2303)	1:95:A:LEU:HD12	1:95:A:LEU:HB2	2	0.24
(1,2303)	1:95:A:LEU:HD13	1:95:A:LEU:HB2	2	0.24
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG11	2	0.24
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG12	2	0.24
(1,1933)	1:77:A:VAL:HB	1:84:A:VAL:HG13	2	0.24
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	8	0.24
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	8	0.24
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	8	0.24
(1,1225)	1:41:A:GLU:HG2	1:42:A:GLU:H	8	0.24
(1,1225)	1:41:A:GLU:HG3	1:42:A:GLU:H	8	0.24
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	2	0.24
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	2	0.24
(1,1088)	1:36:A:ILE:HG21	1:75:A:PHE:HZ	7	0.24
(1,1088)	1:36:A:ILE:HG22	1:75:A:PHE:HZ	7	0.24
(1,1088)	1:36:A:ILE:HG23	1:75:A:PHE:HZ	7	0.24
(1,1054)	1:36:A:ILE:HD11	1:91:A:ASN:H	4	0.24
(1,1054)	1:36:A:ILE:HD12	1:91:A:ASN:H	4	0.24
(1,1054)	1:36:A:ILE:HD13	1:91:A:ASN:H	4	0.24
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	2	0.24
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	2	0.24
(1,826)	1:25:A:PHE:HD1	1:25:A:PHE:H	4	0.24
(1,826)	1:25:A:PHE:HD2	1:25:A:PHE:H	4	0.24
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	4	0.24
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	4	0.24
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	4	0.24
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	4	0.24
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	4	0.24
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	4	0.24
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	4	0.24
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	4	0.24
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	8	0.24
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	8	0.24
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	8	0.24
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	8	0.24
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	8	0.24
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	8	0.24
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	8	0.24
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	8	0.24
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	8	0.24
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	8	0.24
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	8	0.24
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	8	0.24
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	8	0.24
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	8	0.24
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	8	0.24
(1,668)	1:22:A:ILE:HG21	1:52:A:PHE:HA	4	0.24
(1,668)	1:22:A:ILE:HG22	1:52:A:PHE:HA	4	0.24
(1,668)	1:22:A:ILE:HG23	1:52:A:PHE:HA	4	0.24
(1,654)	1:22:A:ILE:HD11	1:75:A:PHE:HB3	8	0.24
(1,654)	1:22:A:ILE:HD12	1:75:A:PHE:HB3	8	0.24
(1,654)	1:22:A:ILE:HD13	1:75:A:PHE:HB3	8	0.24
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD11	9	0.24
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD12	9	0.24
(1,304)	1:14:A:ILE:HA	1:14:A:ILE:HD13	9	0.24
(1,245)	1:11:A:PHE:HZ	1:15:A:ILE:HD11	3	0.24
(1,245)	1:11:A:PHE:HZ	1:15:A:ILE:HD12	3	0.24
(1,245)	1:11:A:PHE:HZ	1:15:A:ILE:HD13	3	0.24
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG11	5	0.24
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG12	5	0.24
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG13	5	0.24
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG11	5	0.24
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG12	5	0.24
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG13	5	0.24
(1,112)	1:6:A:THR:H	1:6:A:THR:HG21	7	0.24
(1,112)	1:6:A:THR:H	1:6:A:THR:HG22	7	0.24
(1,112)	1:6:A:THR:H	1:6:A:THR:HG23	7	0.24
(2,219)	1:43:A:CYS:HB3	1:52:A:PHE:HD1	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,219)	1:43:A:CYS:HB3	1:52:A:PHE:HD2	2	0.23
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	8	0.23
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	8	0.23
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	8	0.23
(1,2388)	1:98:A:LEU:HD21	1:99:A:ILE:HA	1	0.23
(1,2388)	1:98:A:LEU:HD22	1:99:A:ILE:HA	1	0.23
(1,2388)	1:98:A:LEU:HD23	1:99:A:ILE:HA	1	0.23
(1,2383)	1:98:A:LEU:HD11	1:102:A:TYR:HE1	6	0.23
(1,2383)	1:98:A:LEU:HD11	1:102:A:TYR:HE2	6	0.23
(1,2383)	1:98:A:LEU:HD12	1:102:A:TYR:HE1	6	0.23
(1,2383)	1:98:A:LEU:HD12	1:102:A:TYR:HE2	6	0.23
(1,2383)	1:98:A:LEU:HD13	1:102:A:TYR:HE1	6	0.23
(1,2383)	1:98:A:LEU:HD13	1:102:A:TYR:HE2	6	0.23
(1,2200)	1:88:A:LEU:HD21	1:88:A:LEU:HA	3	0.23
(1,2200)	1:88:A:LEU:HD22	1:88:A:LEU:HA	3	0.23
(1,2200)	1:88:A:LEU:HD23	1:88:A:LEU:HA	3	0.23
(1,2172)	1:87:A:LEU:HD11	1:91:A:ASN:HB2	4	0.23
(1,2172)	1:87:A:LEU:HD12	1:91:A:ASN:HB2	4	0.23
(1,2172)	1:87:A:LEU:HD13	1:91:A:ASN:HB2	4	0.23
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG11	1	0.23
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG12	1	0.23
(1,1950)	1:77:A:VAL:HG11	1:84:A:VAL:HG13	1	0.23
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG11	1	0.23
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG12	1	0.23
(1,1950)	1:77:A:VAL:HG12	1:84:A:VAL:HG13	1	0.23
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG11	1	0.23
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG12	1	0.23
(1,1950)	1:77:A:VAL:HG13	1:84:A:VAL:HG13	1	0.23
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	7	0.23
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	7	0.23
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	7	0.23
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD11	10	0.23
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD12	10	0.23
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD13	10	0.23
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	3	0.23
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	3	0.23
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	3	0.23
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	2	0.23
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	2	0.23
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	2	0.23
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	3	0.23
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	3	0.23
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD1	1	0.23
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD2	1	0.23
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD1	1	0.23
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD2	1	0.23
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD1	1	0.23
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD2	1	0.23
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	2	0.23
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	2	0.23
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	2	0.23
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	2	0.23
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	2	0.23
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	2	0.23
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	3	0.23
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	3	0.23
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	3	0.23
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	3	0.23
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	3	0.23
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	3	0.23
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG21	1	0.23
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG22	1	0.23
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG23	1	0.23
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	2	0.23
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	2	0.23
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	2	0.23
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB1	1	0.23
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB2	1	0.23
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB3	1	0.23
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	7	0.23
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	7	0.23
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	9	0.23
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	9	0.23
(1,902)	1:26:A:PHE:HE1	1:54:A:LYS:HG3	9	0.23
(1,902)	1:26:A:PHE:HE2	1:54:A:LYS:HG3	9	0.23
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	9	0.23
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	9	0.23
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	9	0.23
(1,720)	1:23:A:VAL:HG11	1:54:A:LYS:HA	1	0.23
(1,720)	1:23:A:VAL:HG12	1:54:A:LYS:HA	1	0.23
(1,720)	1:23:A:VAL:HG13	1:54:A:LYS:HA	1	0.23
(1,668)	1:22:A:ILE:HG21	1:52:A:PHE:HA	8	0.23
(1,668)	1:22:A:ILE:HG22	1:52:A:PHE:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:22:A:ILE:HG23	1:52:A:PHE:HA	8	0.23
(1,665)	1:22:A:ILE:HG21	1:50:A:MET:HB3	4	0.23
(1,665)	1:22:A:ILE:HG22	1:50:A:MET:HB3	4	0.23
(1,665)	1:22:A:ILE:HG23	1:50:A:MET:HB3	4	0.23
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG21	4	0.23
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG22	4	0.23
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG23	4	0.23
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	1	0.22
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	1	0.22
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	1	0.22
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE1	2	0.22
(2,244)	1:47:A:TYR:HA	1:52:A:PHE:HE2	2	0.22
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	1	0.22
(2,100)	1:21:A:VAL:HA	1:50:A:MET:HB3	4	0.22
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	5	0.22
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	5	0.22
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	5	0.22
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	5	0.22
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	5	0.22
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	5	0.22
(1,1737)	1:69:A:ILE:HD11	1:69:A:ILE:HA	8	0.22
(1,1737)	1:69:A:ILE:HD12	1:69:A:ILE:HA	8	0.22
(1,1737)	1:69:A:ILE:HD13	1:69:A:ILE:HA	8	0.22
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	3	0.22
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	3	0.22
(1,1396)	1:47:A:TYR:HE1	1:100:A:GLU:HG2	5	0.22
(1,1396)	1:47:A:TYR:HE2	1:100:A:GLU:HG2	5	0.22
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD21	1	0.22
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD22	1	0.22
(1,1155)	1:39:A:PHE:HD1	1:95:A:LEU:HD23	1	0.22
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD21	1	0.22
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD22	1	0.22
(1,1155)	1:39:A:PHE:HD2	1:95:A:LEU:HD23	1	0.22
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	3	0.22
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	3	0.22
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	3	0.22
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB1	10	0.22
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB2	10	0.22
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB3	10	0.22
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	3	0.22
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	3	0.22
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	5	0.22
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	5	0.22
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	9	0.22
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	9	0.22
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	9	0.22
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	9	0.22
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	9	0.22
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	9	0.22
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	9	0.22
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	9	0.22
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	9	0.22
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	2	0.22
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	2	0.22
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	2	0.22
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	2	0.22
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	2	0.22
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	2	0.22
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	7	0.22
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	7	0.22
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	7	0.22
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	7	0.22
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	7	0.22
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	7	0.22
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	4	0.22
(1,431)	1:15:A:ILE:HG21	1:81:A:GLY:HA2	9	0.22
(1,431)	1:15:A:ILE:HG22	1:81:A:GLY:HA2	9	0.22
(1,431)	1:15:A:ILE:HG23	1:81:A:GLY:HA2	9	0.22
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG11	4	0.22
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG12	4	0.22
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG13	4	0.22
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG11	4	0.22
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG12	4	0.22
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG13	4	0.22
(1,96)	1:5:A:VAL:H	1:5:A:VAL:HB	4	0.22
(1,89)	1:5:A:VAL:HG21	1:7:A:SER:H	9	0.22
(1,89)	1:5:A:VAL:HG22	1:7:A:SER:H	9	0.22
(1,89)	1:5:A:VAL:HG23	1:7:A:SER:H	9	0.22
(2,385)	1:79:A:LYS:HD2	1:81:A:GLY:H	7	0.21
(2,385)	1:79:A:LYS:HD3	1:81:A:GLY:H	7	0.21
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	6	0.21
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	7	0.21
(1,2550)	1:27:A:ALA:HB1	1:30:A:CYS:HB2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2550)	1:27:A:ALA:HB2	1:30:A:CYS:HB2	7	0.21
(1,2550)	1:27:A:ALA:HB3	1:30:A:CYS:HB2	7	0.21
(1,2200)	1:88:A:LEU:HD21	1:88:A:LEU:HA	8	0.21
(1,2200)	1:88:A:LEU:HD22	1:88:A:LEU:HA	8	0.21
(1,2200)	1:88:A:LEU:HD23	1:88:A:LEU:HA	8	0.21
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB1	10	0.21
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB2	10	0.21
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB3	10	0.21
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB1	10	0.21
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB2	10	0.21
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB3	10	0.21
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB1	10	0.21
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB2	10	0.21
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB3	10	0.21
(1,2172)	1:87:A:LEU:HD11	1:91:A:ASN:HB2	1	0.21
(1,2172)	1:87:A:LEU:HD12	1:91:A:ASN:HB2	1	0.21
(1,2172)	1:87:A:LEU:HD13	1:91:A:ASN:HB2	1	0.21
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD11	10	0.21
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD12	10	0.21
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD13	10	0.21
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD21	3	0.21
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD22	3	0.21
(1,1976)	1:77:A:VAL:HG21	1:98:A:LEU:HD23	3	0.21
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD21	3	0.21
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD22	3	0.21
(1,1976)	1:77:A:VAL:HG22	1:98:A:LEU:HD23	3	0.21
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD21	3	0.21
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD22	3	0.21
(1,1976)	1:77:A:VAL:HG23	1:98:A:LEU:HD23	3	0.21
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	9	0.21
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	9	0.21
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	9	0.21
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	1	0.21
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	1	0.21
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	1	0.21
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	1	0.21
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	1	0.21
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	1	0.21
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	1	0.21
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	1	0.21
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	1	0.21
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG21	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG22	3	0.21
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG23	3	0.21
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	9	0.21
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	9	0.21
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	9	0.21
(1,1550)	1:57:A:VAL:HG21	1:58:A:ASP:H	8	0.21
(1,1550)	1:57:A:VAL:HG22	1:58:A:ASP:H	8	0.21
(1,1550)	1:57:A:VAL:HG23	1:58:A:ASP:H	8	0.21
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	5	0.21
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	5	0.21
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	5	0.21
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB1	4	0.21
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB2	4	0.21
(1,1359)	1:47:A:TYR:HB3	1:103:A:ALA:HB3	4	0.21
(1,1336)	1:46:A:THR:HG21	1:47:A:TYR:H	8	0.21
(1,1336)	1:46:A:THR:HG22	1:47:A:TYR:H	8	0.21
(1,1336)	1:46:A:THR:HG23	1:47:A:TYR:H	8	0.21
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	8	0.21
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	8	0.21
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	8	0.21
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	9	0.21
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	9	0.21
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	9	0.21
(1,1079)	1:36:A:ILE:HG21	1:37:A:ALA:H	6	0.21
(1,1079)	1:36:A:ILE:HG22	1:37:A:ALA:H	6	0.21
(1,1079)	1:36:A:ILE:HG23	1:37:A:ALA:H	6	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	3	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	3	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	3	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	5	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	5	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	5	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	8	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	8	0.21
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	8	0.21
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	1	0.21
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	1	0.21
(1,838)	1:25:A:PHE:HE1	1:63:A:VAL:HG11	4	0.21
(1,838)	1:25:A:PHE:HE1	1:63:A:VAL:HG12	4	0.21
(1,838)	1:25:A:PHE:HE1	1:63:A:VAL:HG13	4	0.21
(1,838)	1:25:A:PHE:HE2	1:63:A:VAL:HG11	4	0.21
(1,838)	1:25:A:PHE:HE2	1:63:A:VAL:HG12	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:25:A:PHE:HE2	1:63:A:VAL:HG13	4	0.21
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	6	0.21
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	6	0.21
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	6	0.21
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	6	0.21
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	6	0.21
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	6	0.21
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	6	0.21
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	6	0.21
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	6	0.21
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	6	0.21
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	6	0.21
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	6	0.21
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	10	0.21
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	10	0.21
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	10	0.21
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	10	0.21
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	10	0.21
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	10	0.21
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	10	0.21
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	10	0.21
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	10	0.21
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	7	0.21
(1,380)	1:15:A:ILE:HD11	1:23:A:VAL:HB	5	0.21
(1,380)	1:15:A:ILE:HD12	1:23:A:VAL:HB	5	0.21
(1,380)	1:15:A:ILE:HD13	1:23:A:VAL:HB	5	0.21
(1,96)	1:5:A:VAL:H	1:5:A:VAL:HB	6	0.21
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE1	8	0.2
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE2	8	0.2
(2,329)	1:69:A:ILE:HG21	1:72:A:MET:HE3	8	0.2
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE1	8	0.2
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE2	8	0.2
(2,329)	1:69:A:ILE:HG22	1:72:A:MET:HE3	8	0.2
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE1	8	0.2
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE2	8	0.2
(2,329)	1:69:A:ILE:HG23	1:72:A:MET:HE3	8	0.2
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	9	0.2
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	9	0.2
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	9	0.2
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE1	6	0.2
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE2	6	0.2
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	5	0.2
(2,151)	1:27:A:ALA:HB1	1:58:A:ASP:HB2	5	0.2
(2,151)	1:27:A:ALA:HB2	1:58:A:ASP:HB2	5	0.2
(2,151)	1:27:A:ALA:HB3	1:58:A:ASP:HB2	5	0.2
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	8	0.2
(1,2542)	1:26:A:PHE:HE1	1:55:A:VAL:HA	9	0.2
(1,2542)	1:26:A:PHE:HE2	1:55:A:VAL:HA	9	0.2
(1,2415)	1:99:A:ILE:HD11	1:103:A:ALA:H	1	0.2
(1,2415)	1:99:A:ILE:HD12	1:103:A:ALA:H	1	0.2
(1,2415)	1:99:A:ILE:HD13	1:103:A:ALA:H	1	0.2
(1,2200)	1:88:A:LEU:HD21	1:88:A:LEU:HA	10	0.2
(1,2200)	1:88:A:LEU:HD22	1:88:A:LEU:HA	10	0.2
(1,2200)	1:88:A:LEU:HD23	1:88:A:LEU:HA	10	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD11	6	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD12	6	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD13	6	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD11	9	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD12	9	0.2
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD13	9	0.2
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG21	2	0.2
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG22	2	0.2
(1,2135)	1:85:A:ASP:HA	1:86:A:THR:HG23	2	0.2
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	2	0.2
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	2	0.2
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	2	0.2
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	5	0.2
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	5	0.2
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	5	0.2
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	6	0.2
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	6	0.2
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	6	0.2
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	8	0.2
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	8	0.2
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	8	0.2
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	2	0.2
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	2	0.2
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	2	0.2
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	3	0.2
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	3	0.2
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	3	0.2
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	8	0.2
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	8	0.2
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	9	0.2
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	9	0.2
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	9	0.2
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	1	0.2
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	1	0.2
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	1	0.2
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	1	0.2
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	1	0.2
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	1	0.2
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	1	0.2
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	1	0.2
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	1	0.2
(1,1505)	1:54:A:LYS:HA	1:54:A:LYS:HG3	10	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	3	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	3	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	3	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	6	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	6	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	6	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	8	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	8	0.2
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	8	0.2
(1,1336)	1:46:A:THR:HG21	1:47:A:TYR:H	7	0.2
(1,1336)	1:46:A:THR:HG22	1:47:A:TYR:H	7	0.2
(1,1336)	1:46:A:THR:HG23	1:47:A:TYR:H	7	0.2
(1,1331)	1:46:A:THR:HG21	1:47:A:TYR:HA	5	0.2
(1,1331)	1:46:A:THR:HG22	1:47:A:TYR:HA	5	0.2
(1,1331)	1:46:A:THR:HG23	1:47:A:TYR:HA	5	0.2
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	5	0.2
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	5	0.2
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	5	0.2
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	3	0.2
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	3	0.2
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	4	0.2
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	4	0.2
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB1	4	0.2
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB2	4	0.2
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB3	4	0.2
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	2	0.2
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	2	0.2
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG21	6	0.2
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG22	6	0.2
(1,503)	1:18:A:ASN:HD21	1:21:A:VAL:HG23	6	0.2
(1,431)	1:15:A:ILE:HG21	1:81:A:GLY:HA2	3	0.2
(1,431)	1:15:A:ILE:HG22	1:81:A:GLY:HA2	3	0.2
(1,431)	1:15:A:ILE:HG23	1:81:A:GLY:HA2	3	0.2
(1,380)	1:15:A:ILE:HD11	1:23:A:VAL:HB	8	0.2
(1,380)	1:15:A:ILE:HD12	1:23:A:VAL:HB	8	0.2
(1,380)	1:15:A:ILE:HD13	1:23:A:VAL:HB	8	0.2
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE1	4	0.19
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE2	4	0.19
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE3	4	0.19
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	2	0.19
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	4	0.19
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	8	0.19
(1,2468)	1:101:A:LYS:HB2	1:103:A:ALA:H	4	0.19
(1,2468)	1:101:A:LYS:HB2	1:103:A:ALA:H	5	0.19
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE1	4	0.19
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE2	4	0.19
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE1	4	0.19
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE2	4	0.19
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE1	4	0.19
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE2	4	0.19
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	6	0.19
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	6	0.19
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	6	0.19
(1,1915)	1:76:A:LYS:HD2	1:86:A:THR:HA	2	0.19
(1,1915)	1:76:A:LYS:HD3	1:86:A:THR:HA	2	0.19
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	4	0.19
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	4	0.19
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	4	0.19
(1,1634)	1:63:A:VAL:HG11	1:67:A:GLU:HG2	8	0.19
(1,1634)	1:63:A:VAL:HG11	1:67:A:GLU:HG3	8	0.19
(1,1634)	1:63:A:VAL:HG12	1:67:A:GLU:HG2	8	0.19
(1,1634)	1:63:A:VAL:HG12	1:67:A:GLU:HG3	8	0.19
(1,1634)	1:63:A:VAL:HG13	1:67:A:GLU:HG2	8	0.19
(1,1634)	1:63:A:VAL:HG13	1:67:A:GLU:HG3	8	0.19
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	1	0.19
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	1	0.19
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	1	0.19
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	9	0.19
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	9	0.19
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD1	9	0.19
(1,1334)	1:46:A:THR:HG21	1:47:A:TYR:HD2	9	0.19
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD1	9	0.19
(1,1334)	1:46:A:THR:HG22	1:47:A:TYR:HD2	9	0.19
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD1	9	0.19
(1,1334)	1:46:A:THR:HG23	1:47:A:TYR:HD2	9	0.19
(1,1331)	1:46:A:THR:HG21	1:47:A:TYR:HA	8	0.19
(1,1331)	1:46:A:THR:HG22	1:47:A:TYR:HA	8	0.19
(1,1331)	1:46:A:THR:HG23	1:47:A:TYR:HA	8	0.19
(1,1225)	1:41:A:GLU:HG2	1:42:A:GLU:H	3	0.19
(1,1225)	1:41:A:GLU:HG3	1:42:A:GLU:H	3	0.19
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG21	5	0.19
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG22	5	0.19
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG23	5	0.19
(1,1079)	1:36:A:ILE:HG21	1:37:A:ALA:H	3	0.19
(1,1079)	1:36:A:ILE:HG22	1:37:A:ALA:H	3	0.19
(1,1079)	1:36:A:ILE:HG23	1:37:A:ALA:H	3	0.19
(1,900)	1:26:A:PHE:HE1	1:54:A:LYS:HB2	4	0.19
(1,900)	1:26:A:PHE:HE1	1:54:A:LYS:HB3	4	0.19
(1,900)	1:26:A:PHE:HE2	1:54:A:LYS:HB2	4	0.19
(1,900)	1:26:A:PHE:HE2	1:54:A:LYS:HB3	4	0.19
(1,841)	1:25:A:PHE:HE1	1:69:A:ILE:HD11	2	0.19
(1,841)	1:25:A:PHE:HE1	1:69:A:ILE:HD12	2	0.19
(1,841)	1:25:A:PHE:HE1	1:69:A:ILE:HD13	2	0.19
(1,841)	1:25:A:PHE:HE2	1:69:A:ILE:HD11	2	0.19
(1,841)	1:25:A:PHE:HE2	1:69:A:ILE:HD12	2	0.19
(1,841)	1:25:A:PHE:HE2	1:69:A:ILE:HD13	2	0.19
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	10	0.19
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG11	3	0.19
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG12	3	0.19
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG13	3	0.19
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	9	0.19
(1,425)	1:15:A:ILE:HG21	1:78:A:TYR:HB2	8	0.19
(1,425)	1:15:A:ILE:HG22	1:78:A:TYR:HB2	8	0.19
(1,425)	1:15:A:ILE:HG23	1:78:A:TYR:HB2	8	0.19
(1,343)	1:14:A:ILE:HG21	1:18:A:ASN:HD22	9	0.19
(1,343)	1:14:A:ILE:HG22	1:18:A:ASN:HD22	9	0.19
(1,343)	1:14:A:ILE:HG23	1:18:A:ASN:HD22	9	0.19
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG2	6	0.19
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG3	6	0.19
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG21	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG22	5	0.19
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG23	5	0.19
(1,105)	1:5:A:VAL:H	1:55:A:VAL:HB	1	0.19
(1,96)	1:5:A:VAL:H	1:5:A:VAL:HB	5	0.19
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	5	0.18
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	5	0.18
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	6	0.18
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	6	0.18
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE1	10	0.18
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE2	10	0.18
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	6	0.18
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	6	0.18
(2,243)	1:47:A:TYR:HA	1:50:A:MET:HB2	8	0.18
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE1	3	0.18
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE2	3	0.18
(2,183)	1:29:A:TRP:HE1	1:72:A:MET:HE3	3	0.18
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	1	0.18
(1,2542)	1:26:A:PHE:HE1	1:55:A:VAL:HA	7	0.18
(1,2542)	1:26:A:PHE:HE2	1:55:A:VAL:HA	7	0.18
(1,2535)	1:103:A:ALA:H	1:104:A:ALA:HA	1	0.18
(1,2197)	1:88:A:LEU:HD11	1:89:A:GLY:H	10	0.18
(1,2197)	1:88:A:LEU:HD12	1:89:A:GLY:H	10	0.18
(1,2197)	1:88:A:LEU:HD13	1:89:A:GLY:H	10	0.18
(1,2197)	1:88:A:LEU:HD21	1:89:A:GLY:H	10	0.18
(1,2197)	1:88:A:LEU:HD22	1:89:A:GLY:H	10	0.18
(1,2197)	1:88:A:LEU:HD23	1:89:A:GLY:H	10	0.18
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE1	2	0.18
(1,2127)	1:84:A:VAL:HG21	1:102:A:TYR:HE2	2	0.18
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE1	2	0.18
(1,2127)	1:84:A:VAL:HG22	1:102:A:TYR:HE2	2	0.18
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE1	2	0.18
(1,2127)	1:84:A:VAL:HG23	1:102:A:TYR:HE2	2	0.18
(1,1969)	1:77:A:VAL:HG21	1:85:A:ASP:HB3	6	0.18
(1,1969)	1:77:A:VAL:HG22	1:85:A:ASP:HB3	6	0.18
(1,1969)	1:77:A:VAL:HG23	1:85:A:ASP:HB3	6	0.18
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	1	0.18
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	1	0.18
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	1	0.18
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	5	0.18
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	5	0.18
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	5	0.18
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	10	0.18
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	10	0.18
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	1	0.18
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	1	0.18
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	1	0.18
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	8	0.18
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	8	0.18
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	8	0.18
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG21	7	0.18
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG22	7	0.18
(1,1413)	1:48:A:THR:H	1:48:A:THR:HG23	7	0.18
(1,1336)	1:46:A:THR:HG21	1:47:A:TYR:H	4	0.18
(1,1336)	1:46:A:THR:HG22	1:47:A:TYR:H	4	0.18
(1,1336)	1:46:A:THR:HG23	1:47:A:TYR:H	4	0.18
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	2	0.18
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	2	0.18
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	2	0.18
(1,788)	1:24:A:ASP:HB2	1:75:A:PHE:HE1	4	0.18
(1,788)	1:24:A:ASP:HB2	1:75:A:PHE:HE2	4	0.18
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	4	0.18
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	4	0.18
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	4	0.18
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	7	0.18
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	7	0.18
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	7	0.18
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	7	0.18
(1,431)	1:15:A:ILE:HG21	1:81:A:GLY:HA2	6	0.18
(1,431)	1:15:A:ILE:HG22	1:81:A:GLY:HA2	6	0.18
(1,431)	1:15:A:ILE:HG23	1:81:A:GLY:HA2	6	0.18
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD1	3	0.18
(1,144)	1:8:A:GLN:HE21	1:11:A:PHE:HD2	3	0.18
(1,112)	1:6:A:THR:H	1:6:A:THR:HG21	4	0.18
(1,112)	1:6:A:THR:H	1:6:A:THR:HG22	4	0.18
(1,112)	1:6:A:THR:H	1:6:A:THR:HG23	4	0.18
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE1	8	0.17
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE2	8	0.17
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE1	3	0.17
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE2	3	0.17
(2,341)	1:72:A:MET:HA	1:72:A:MET:HE3	3	0.17
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	2	0.17
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	2	0.17
(2,243)	1:47:A:TYR:HA	1:50:A:MET:HB2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	10	0.17
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	4	0.17
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	7	0.17
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB1	10	0.17
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB2	10	0.17
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB3	10	0.17
(1,1959)	1:77:A:VAL:HG11	1:102:A:TYR:HB2	3	0.17
(1,1959)	1:77:A:VAL:HG12	1:102:A:TYR:HB2	3	0.17
(1,1959)	1:77:A:VAL:HG13	1:102:A:TYR:HB2	3	0.17
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	2	0.17
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	2	0.17
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	2	0.17
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	3	0.17
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	3	0.17
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	3	0.17
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	3	0.17
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	3	0.17
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	3	0.17
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	3	0.17
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	3	0.17
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	3	0.17
(1,1550)	1:57:A:VAL:HG21	1:58:A:ASP:H	5	0.17
(1,1550)	1:57:A:VAL:HG22	1:58:A:ASP:H	5	0.17
(1,1550)	1:57:A:VAL:HG23	1:58:A:ASP:H	5	0.17
(1,1488)	1:52:A:PHE:HZ	1:99:A:ILE:HG12	6	0.17
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD11	1	0.17
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD12	1	0.17
(1,1358)	1:47:A:TYR:HB3	1:99:A:ILE:HD13	1	0.17
(1,1336)	1:46:A:THR:HG21	1:47:A:TYR:H	6	0.17
(1,1336)	1:46:A:THR:HG22	1:47:A:TYR:H	6	0.17
(1,1336)	1:46:A:THR:HG23	1:47:A:TYR:H	6	0.17
(1,1331)	1:46:A:THR:HG21	1:47:A:TYR:HA	4	0.17
(1,1331)	1:46:A:THR:HG22	1:47:A:TYR:HA	4	0.17
(1,1331)	1:46:A:THR:HG23	1:47:A:TYR:HA	4	0.17
(1,1331)	1:46:A:THR:HG21	1:47:A:TYR:HA	6	0.17
(1,1331)	1:46:A:THR:HG22	1:47:A:TYR:HA	6	0.17
(1,1331)	1:46:A:THR:HG23	1:47:A:TYR:HA	6	0.17
(1,1331)	1:46:A:THR:HG21	1:47:A:TYR:HA	7	0.17
(1,1331)	1:46:A:THR:HG22	1:47:A:TYR:HA	7	0.17
(1,1331)	1:46:A:THR:HG23	1:47:A:TYR:HA	7	0.17
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	6	0.17
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	8	0.17
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	8	0.17
(1,840)	1:25:A:PHE:HE1	1:67:A:GLU:HG2	8	0.17
(1,840)	1:25:A:PHE:HE1	1:67:A:GLU:HG3	8	0.17
(1,840)	1:25:A:PHE:HE2	1:67:A:GLU:HG2	8	0.17
(1,840)	1:25:A:PHE:HE2	1:67:A:GLU:HG3	8	0.17
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	4	0.17
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	8	0.17
(1,580)	1:20:A:LEU:HD21	1:77:A:VAL:HG11	9	0.17
(1,580)	1:20:A:LEU:HD21	1:77:A:VAL:HG12	9	0.17
(1,580)	1:20:A:LEU:HD21	1:77:A:VAL:HG13	9	0.17
(1,580)	1:20:A:LEU:HD22	1:77:A:VAL:HG11	9	0.17
(1,580)	1:20:A:LEU:HD22	1:77:A:VAL:HG12	9	0.17
(1,580)	1:20:A:LEU:HD22	1:77:A:VAL:HG13	9	0.17
(1,580)	1:20:A:LEU:HD23	1:77:A:VAL:HG11	9	0.17
(1,580)	1:20:A:LEU:HD23	1:77:A:VAL:HG12	9	0.17
(1,580)	1:20:A:LEU:HD23	1:77:A:VAL:HG13	9	0.17
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG11	3	0.17
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG12	3	0.17
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG13	3	0.17
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG11	3	0.17
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG12	3	0.17
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG13	3	0.17
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG11	3	0.17
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG12	3	0.17
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG13	3	0.17
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG2	7	0.17
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG3	7	0.17
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG11	8	0.17
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG12	8	0.17
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG13	8	0.17
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG11	8	0.17
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG12	8	0.17
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG13	8	0.17
(1,153)	1:8:A:GLN:HE22	1:9:A:SER:H	1	0.17
(1,83)	1:5:A:VAL:HG11	1:11:A:PHE:HA	9	0.17
(1,83)	1:5:A:VAL:HG12	1:11:A:PHE:HA	9	0.17
(1,83)	1:5:A:VAL:HG13	1:11:A:PHE:HA	9	0.17
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB1	9	0.16
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB2	9	0.16
(2,394)	1:88:A:LEU:H	1:94:A:ALA:HB3	9	0.16
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE1	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:67:A:GLU:HA	1:78:A:TYR:HE2	3	0.16
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	2	0.16
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	2	0.16
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	2	0.16
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	2	0.16
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	2	0.16
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	1	0.16
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	1	0.16
(2,235)	1:44:A:SER:HG	1:52:A:PHE:HE1	9	0.16
(2,235)	1:44:A:SER:HG	1:52:A:PHE:HE2	9	0.16
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG21	5	0.16
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG22	5	0.16
(2,218)	1:43:A:CYS:HB3	1:46:A:THR:HG23	5	0.16
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	9	0.16
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG2	3	0.16
(2,118)	1:25:A:PHE:HD1	1:67:A:GLU:HG3	3	0.16
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG2	3	0.16
(2,118)	1:25:A:PHE:HD2	1:67:A:GLU:HG3	3	0.16
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	2	0.16
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	2	0.16
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	2	0.16
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	2	0.16
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	8	0.16
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	10	0.16
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	9	0.16
(1,2550)	1:27:A:ALA:HB1	1:30:A:CYS:HB2	1	0.16
(1,2550)	1:27:A:ALA:HB2	1:30:A:CYS:HB2	1	0.16
(1,2550)	1:27:A:ALA:HB3	1:30:A:CYS:HB2	1	0.16
(1,2535)	1:103:A:ALA:H	1:104:A:ALA:HA	6	0.16
(1,2407)	1:99:A:ILE:HA	1:104:A:ALA:H	3	0.16
(1,2407)	1:99:A:ILE:HA	1:104:A:ALA:H	4	0.16
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	2	0.16
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	10	0.16
(1,2168)	1:87:A:LEU:HD11	1:89:A:GLY:H	6	0.16
(1,2168)	1:87:A:LEU:HD12	1:89:A:GLY:H	6	0.16
(1,2168)	1:87:A:LEU:HD13	1:89:A:GLY:H	6	0.16
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD11	3	0.16
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD12	3	0.16
(1,2139)	1:85:A:ASP:HB3	1:98:A:LEU:HD13	3	0.16
(1,1988)	1:77:A:VAL:H	1:84:A:VAL:HB	6	0.16
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE1	6	0.16
(1,1981)	1:77:A:VAL:HG21	1:102:A:TYR:HE2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE1	6	0.16
(1,1981)	1:77:A:VAL:HG22	1:102:A:TYR:HE2	6	0.16
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE1	6	0.16
(1,1981)	1:77:A:VAL:HG23	1:102:A:TYR:HE2	6	0.16
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	3	0.16
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	3	0.16
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	3	0.16
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	7	0.16
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	7	0.16
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	7	0.16
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	3	0.16
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	3	0.16
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	3	0.16
(1,1938)	1:77:A:VAL:HG11	1:77:A:VAL:HA	9	0.16
(1,1938)	1:77:A:VAL:HG12	1:77:A:VAL:HA	9	0.16
(1,1938)	1:77:A:VAL:HG13	1:77:A:VAL:HA	9	0.16
(1,1915)	1:76:A:LYS:HD2	1:86:A:THR:HA	7	0.16
(1,1915)	1:76:A:LYS:HD3	1:86:A:THR:HA	7	0.16
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB1	8	0.16
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB2	8	0.16
(1,1890)	1:75:A:PHE:HZ	1:90:A:ALA:HB3	8	0.16
(1,1816)	1:74:A:THR:HG21	1:74:A:THR:HA	10	0.16
(1,1816)	1:74:A:THR:HG22	1:74:A:THR:HA	10	0.16
(1,1816)	1:74:A:THR:HG23	1:74:A:THR:HA	10	0.16
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	2	0.16
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	2	0.16
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	2	0.16
(1,1737)	1:69:A:ILE:HD11	1:69:A:ILE:HA	4	0.16
(1,1737)	1:69:A:ILE:HD12	1:69:A:ILE:HA	4	0.16
(1,1737)	1:69:A:ILE:HD13	1:69:A:ILE:HA	4	0.16
(1,1737)	1:69:A:ILE:HD11	1:69:A:ILE:HA	5	0.16
(1,1737)	1:69:A:ILE:HD12	1:69:A:ILE:HA	5	0.16
(1,1737)	1:69:A:ILE:HD13	1:69:A:ILE:HA	5	0.16
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD11	1	0.16
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD12	1	0.16
(1,1691)	1:67:A:GLU:HB3	1:69:A:ILE:HD13	1	0.16
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	9	0.16
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	9	0.16
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	9	0.16
(1,1505)	1:54:A:LYS:HA	1:54:A:LYS:HG3	3	0.16
(1,1437)	1:50:A:MET:HG2	1:103:A:ALA:H	7	0.16
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	9	0.16
(1,1225)	1:41:A:GLU:HG2	1:42:A:GLU:H	2	0.16
(1,1225)	1:41:A:GLU:HG3	1:42:A:GLU:H	2	0.16
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG21	3	0.16
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG22	3	0.16
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG23	3	0.16
(1,1079)	1:36:A:ILE:HG21	1:37:A:ALA:H	5	0.16
(1,1079)	1:36:A:ILE:HG22	1:37:A:ALA:H	5	0.16
(1,1079)	1:36:A:ILE:HG23	1:37:A:ALA:H	5	0.16
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	4	0.16
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	4	0.16
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	4	0.16
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	6	0.16
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	9	0.16
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	10	0.16
(1,900)	1:26:A:PHE:HE1	1:54:A:LYS:HB2	5	0.16
(1,900)	1:26:A:PHE:HE1	1:54:A:LYS:HB3	5	0.16
(1,900)	1:26:A:PHE:HE2	1:54:A:LYS:HB2	5	0.16
(1,900)	1:26:A:PHE:HE2	1:54:A:LYS:HB3	5	0.16
(1,848)	1:25:A:PHE:HE1	1:78:A:TYR:HE1	1	0.16
(1,848)	1:25:A:PHE:HE1	1:78:A:TYR:HE2	1	0.16
(1,848)	1:25:A:PHE:HE2	1:78:A:TYR:HE1	1	0.16
(1,848)	1:25:A:PHE:HE2	1:78:A:TYR:HE2	1	0.16
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	1	0.16
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	1	0.16
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	1	0.16
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	1	0.16
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	1	0.16
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	1	0.16
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	1	0.16
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	1	0.16
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	1	0.16
(1,724)	1:23:A:VAL:HG11	1:55:A:VAL:H	1	0.16
(1,724)	1:23:A:VAL:HG12	1:55:A:VAL:H	1	0.16
(1,724)	1:23:A:VAL:HG13	1:55:A:VAL:H	1	0.16
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	1	0.16
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	9	0.16
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	6	0.16
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG11	2	0.16
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG12	2	0.16
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG13	2	0.16
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG11	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG12	2	0.16
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG13	2	0.16
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG11	2	0.16
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG12	2	0.16
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG13	2	0.16
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG11	2	0.16
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG12	2	0.16
(1,227)	1:11:A:PHE:HE1	1:23:A:VAL:HG13	2	0.16
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG11	2	0.16
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG12	2	0.16
(1,227)	1:11:A:PHE:HE2	1:23:A:VAL:HG13	2	0.16
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG11	8	0.16
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG12	8	0.16
(1,168)	1:8:A:GLN:H	1:60:A:VAL:HG13	8	0.16
(1,153)	1:8:A:GLN:HE22	1:9:A:SER:H	3	0.16
(1,153)	1:8:A:GLN:HE22	1:9:A:SER:H	8	0.16
(2,327)	1:69:A:ILE:HG21	1:72:A:MET:HB3	4	0.15
(2,327)	1:69:A:ILE:HG22	1:72:A:MET:HB3	4	0.15
(2,327)	1:69:A:ILE:HG23	1:72:A:MET:HB3	4	0.15
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD1	10	0.15
(2,266)	1:50:A:MET:H	1:52:A:PHE:HD2	10	0.15
(2,264)	1:50:A:MET:HE1	1:99:A:ILE:HA	4	0.15
(2,264)	1:50:A:MET:HE2	1:99:A:ILE:HA	4	0.15
(2,264)	1:50:A:MET:HE3	1:99:A:ILE:HA	4	0.15
(2,157)	1:27:A:ALA:H	1:30:A:CYS:H	3	0.15
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	10	0.15
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	10	0.15
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	10	0.15
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	10	0.15
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	2	0.15
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	3	0.15
(2,19)	1:2:A:VAL:HB	1:3:A:LYS:HA	4	0.15
(1,2542)	1:26:A:PHE:HE1	1:55:A:VAL:HA	8	0.15
(1,2542)	1:26:A:PHE:HE2	1:55:A:VAL:HA	8	0.15
(1,2535)	1:103:A:ALA:H	1:104:A:ALA:HA	3	0.15
(1,2506)	1:101:A:LYS:H	1:103:A:ALA:H	2	0.15
(1,2407)	1:99:A:ILE:HA	1:104:A:ALA:H	1	0.15
(1,2407)	1:99:A:ILE:HA	1:104:A:ALA:H	8	0.15
(1,2407)	1:99:A:ILE:HA	1:104:A:ALA:H	10	0.15
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	3	0.15
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	4	0.15
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	8	0.15
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	9	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	1	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	2	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	3	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	4	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	5	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	6	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	7	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	8	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	9	0.15
(1,2243)	1:91:A:ASN:HD21	1:91:A:ASN:HD22	10	0.15
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB1	1	0.15
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB2	1	0.15
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB3	1	0.15
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB1	1	0.15
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB2	1	0.15
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB3	1	0.15
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB1	1	0.15
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB2	1	0.15
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB3	1	0.15
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	7	0.15
(1,2054)	1:79:A:LYS:HE2	1:80:A:ASN:HD22	4	0.15
(1,2054)	1:79:A:LYS:HE3	1:80:A:ASN:HD22	4	0.15
(1,1988)	1:77:A:VAL:H	1:84:A:VAL:HB	7	0.15
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	4	0.15
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	4	0.15
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	4	0.15
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	4	0.15
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	4	0.15
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	4	0.15
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	4	0.15
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	4	0.15
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	4	0.15
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD11	4	0.15
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD12	4	0.15
(1,1693)	1:67:A:GLU:HB2	1:69:A:ILE:HD13	4	0.15
(1,1689)	1:66:A:LYS:H	1:66:A:LYS:HG2	10	0.15
(1,1689)	1:66:A:LYS:H	1:66:A:LYS:HG3	10	0.15
(1,1685)	1:66:A:LYS:HG2	1:67:A:GLU:H	8	0.15
(1,1685)	1:66:A:LYS:HG3	1:67:A:GLU:H	8	0.15
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	1	0.15
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	1	0.15
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	4	0.15
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	4	0.15
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	4	0.15
(1,1550)	1:57:A:VAL:HG21	1:58:A:ASP:H	9	0.15
(1,1550)	1:57:A:VAL:HG22	1:58:A:ASP:H	9	0.15
(1,1550)	1:57:A:VAL:HG23	1:58:A:ASP:H	9	0.15
(1,1433)	1:50:A:MET:HG3	1:103:A:ALA:H	1	0.15
(1,1399)	1:47:A:TYR:HE1	1:104:A:ALA:HB1	6	0.15
(1,1399)	1:47:A:TYR:HE1	1:104:A:ALA:HB2	6	0.15
(1,1399)	1:47:A:TYR:HE1	1:104:A:ALA:HB3	6	0.15
(1,1399)	1:47:A:TYR:HE2	1:104:A:ALA:HB1	6	0.15
(1,1399)	1:47:A:TYR:HE2	1:104:A:ALA:HB2	6	0.15
(1,1399)	1:47:A:TYR:HE2	1:104:A:ALA:HB3	6	0.15
(1,1225)	1:41:A:GLU:HG2	1:42:A:GLU:H	6	0.15
(1,1225)	1:41:A:GLU:HG3	1:42:A:GLU:H	6	0.15
(1,1218)	1:40:A:TYR:H	1:92:A:ASP:HA	4	0.15
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	1	0.15
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	1	0.15
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	5	0.15
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	5	0.15
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG21	8	0.15
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG22	8	0.15
(1,1097)	1:36:A:ILE:H	1:36:A:ILE:HG23	8	0.15
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	5	0.15
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	5	0.15
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	6	0.15
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	6	0.15
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	8	0.15
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	8	0.15
(1,780)	1:24:A:ASP:HB3	1:26:A:PHE:H	4	0.15
(1,753)	1:23:A:VAL:HG21	1:55:A:VAL:H	2	0.15
(1,753)	1:23:A:VAL:HG22	1:55:A:VAL:H	2	0.15
(1,753)	1:23:A:VAL:HG23	1:55:A:VAL:H	2	0.15
(1,746)	1:23:A:VAL:HG21	1:53:A:ILE:HG13	10	0.15
(1,746)	1:23:A:VAL:HG22	1:53:A:ILE:HG13	10	0.15
(1,746)	1:23:A:VAL:HG23	1:53:A:ILE:HG13	10	0.15
(1,736)	1:23:A:VAL:HG21	1:24:A:ASP:H	3	0.15
(1,736)	1:23:A:VAL:HG22	1:24:A:ASP:H	3	0.15
(1,736)	1:23:A:VAL:HG23	1:24:A:ASP:H	3	0.15
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	10	0.15
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	10	0.15
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	4	0.15
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	4	0.15
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	4	0.15
(1,425)	1:15:A:ILE:HG21	1:78:A:TYR:HB2	3	0.15
(1,425)	1:15:A:ILE:HG22	1:78:A:TYR:HB2	3	0.15
(1,425)	1:15:A:ILE:HG23	1:78:A:TYR:HB2	3	0.15
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	1	0.15
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	2	0.15
(1,381)	1:15:A:ILE:HD11	1:23:A:VAL:HG11	3	0.15
(1,381)	1:15:A:ILE:HD11	1:23:A:VAL:HG12	3	0.15
(1,381)	1:15:A:ILE:HD11	1:23:A:VAL:HG13	3	0.15
(1,381)	1:15:A:ILE:HD12	1:23:A:VAL:HG11	3	0.15
(1,381)	1:15:A:ILE:HD12	1:23:A:VAL:HG12	3	0.15
(1,381)	1:15:A:ILE:HD12	1:23:A:VAL:HG13	3	0.15
(1,381)	1:15:A:ILE:HD13	1:23:A:VAL:HG11	3	0.15
(1,381)	1:15:A:ILE:HD13	1:23:A:VAL:HG12	3	0.15
(1,381)	1:15:A:ILE:HD13	1:23:A:VAL:HG13	3	0.15
(1,380)	1:15:A:ILE:HD11	1:23:A:VAL:HB	3	0.15
(1,380)	1:15:A:ILE:HD12	1:23:A:VAL:HB	3	0.15
(1,380)	1:15:A:ILE:HD13	1:23:A:VAL:HB	3	0.15
(1,380)	1:15:A:ILE:HD11	1:23:A:VAL:HB	7	0.15
(1,380)	1:15:A:ILE:HD12	1:23:A:VAL:HB	7	0.15
(1,380)	1:15:A:ILE:HD13	1:23:A:VAL:HB	7	0.15
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG21	9	0.15
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG22	9	0.15
(1,106)	1:5:A:VAL:H	1:55:A:VAL:HG23	9	0.15
(2,385)	1:79:A:LYS:HD2	1:81:A:GLY:H	5	0.14
(2,385)	1:79:A:LYS:HD3	1:81:A:GLY:H	5	0.14
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	6	0.14
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	1	0.14
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	10	0.14
(2,79)	1:12:A:ASP:HB3	1:66:A:LYS:HD2	4	0.14
(2,79)	1:12:A:ASP:HB3	1:66:A:LYS:HD3	4	0.14
(1,2506)	1:101:A:LYS:H	1:103:A:ALA:H	7	0.14
(1,2473)	1:101:A:LYS:HE2	1:101:A:LYS:HG3	10	0.14
(1,2473)	1:101:A:LYS:HE3	1:101:A:LYS:HG3	10	0.14
(1,2463)	1:101:A:LYS:HA	1:104:A:ALA:H	5	0.14
(1,2407)	1:99:A:ILE:HA	1:104:A:ALA:H	6	0.14
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	1	0.14
(1,2396)	1:98:A:LEU:H	1:98:A:LEU:HG	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	8	0.14
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	10	0.14
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	10	0.14
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	10	0.14
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	10	0.14
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	10	0.14
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	10	0.14
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	10	0.14
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	10	0.14
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	10	0.14
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	10	0.14
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	10	0.14
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	10	0.14
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	4	0.14
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	4	0.14
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	4	0.14
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	5	0.14
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	5	0.14
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	5	0.14
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	8	0.14
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	8	0.14
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	8	0.14
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	8	0.14
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	8	0.14
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	8	0.14
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	8	0.14
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	8	0.14
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	8	0.14
(1,1737)	1:69:A:ILE:HD11	1:69:A:ILE:HA	10	0.14
(1,1737)	1:69:A:ILE:HD12	1:69:A:ILE:HA	10	0.14
(1,1737)	1:69:A:ILE:HD13	1:69:A:ILE:HA	10	0.14
(1,1703)	1:67:A:GLU:H	1:68:A:ASN:HB2	7	0.14
(1,1703)	1:67:A:GLU:H	1:68:A:ASN:HB2	8	0.14
(1,1607)	1:62:A:GLU:HB3	1:63:A:VAL:H	2	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	2	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	2	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	2	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	7	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	7	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	7	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	8	0.14
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	8	0.14
(1,1486)	1:52:A:PHE:HZ	1:99:A:ILE:HA	3	0.14
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG21	6	0.14
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG22	6	0.14
(1,1267)	1:43:A:CYS:HB3	1:99:A:ILE:HG23	6	0.14
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD21	10	0.14
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD22	10	0.14
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD23	10	0.14
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD21	10	0.14
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD22	10	0.14
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD23	10	0.14
(1,1167)	1:39:A:PHE:HE1	1:95:A:LEU:HD21	10	0.14
(1,1167)	1:39:A:PHE:HE1	1:95:A:LEU:HD22	10	0.14
(1,1167)	1:39:A:PHE:HE1	1:95:A:LEU:HD23	10	0.14
(1,1167)	1:39:A:PHE:HE2	1:95:A:LEU:HD21	10	0.14
(1,1167)	1:39:A:PHE:HE2	1:95:A:LEU:HD22	10	0.14
(1,1167)	1:39:A:PHE:HE2	1:95:A:LEU:HD23	10	0.14
(1,1133)	1:39:A:PHE:HB2	1:41:A:GLU:H	10	0.14
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB1	8	0.14
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB2	8	0.14
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB3	8	0.14
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD1	6	0.14
(1,913)	1:26:A:PHE:H	1:26:A:PHE:HD2	6	0.14
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG21	8	0.14
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG22	8	0.14
(1,684)	1:22:A:ILE:H	1:22:A:ILE:HG23	8	0.14
(1,668)	1:22:A:ILE:HG21	1:52:A:PHE:HA	1	0.14
(1,668)	1:22:A:ILE:HG22	1:52:A:PHE:HA	1	0.14
(1,668)	1:22:A:ILE:HG23	1:52:A:PHE:HA	1	0.14
(1,654)	1:22:A:ILE:HD11	1:75:A:PHE:HB3	6	0.14
(1,654)	1:22:A:ILE:HD12	1:75:A:PHE:HB3	6	0.14
(1,654)	1:22:A:ILE:HD13	1:75:A:PHE:HB3	6	0.14
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	3	0.14
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	6	0.14
(1,611)	1:21:A:VAL:HB	1:78:A:TYR:HB3	9	0.14
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	3	0.14
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG11	7	0.14
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG12	7	0.14
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG13	7	0.14
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG11	10	0.14
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG12	10	0.14
(1,587)	1:20:A:LEU:HG	1:77:A:VAL:HG13	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:20:A:LEU:HG	1:51:A:VAL:H	7	0.14
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	7	0.14
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	10	0.14
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	5	0.14
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	6	0.14
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	7	0.14
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	9	0.14
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG2	2	0.14
(1,252)	1:11:A:PHE:HZ	1:67:A:GLU:HG3	2	0.14
(1,44)	1:3:A:LYS:HG3	1:53:A:ILE:HA	4	0.14
(2,373)	1:77:A:VAL:H	1:83:A:SER:HA	6	0.13
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	1	0.13
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	1	0.13
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	3	0.13
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	3	0.13
(2,243)	1:47:A:TYR:HA	1:50:A:MET:HB2	10	0.13
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD1	4	0.13
(2,224)	1:43:A:CYS:HB2	1:52:A:PHE:HD2	4	0.13
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE2	4	0.13
(2,99)	1:20:A:LEU:HA	1:79:A:LYS:HE3	4	0.13
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE2	4	0.13
(2,98)	1:20:A:LEU:HA	1:79:A:LYS:HE3	4	0.13
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	3	0.13
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	5	0.13
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	2	0.13
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	5	0.13
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	6	0.13
(1,2535)	1:103:A:ALA:H	1:104:A:ALA:HA	10	0.13
(1,2506)	1:101:A:LYS:H	1:103:A:ALA:H	5	0.13
(1,2473)	1:101:A:LYS:HE2	1:101:A:LYS:HG3	7	0.13
(1,2473)	1:101:A:LYS:HE3	1:101:A:LYS:HG3	7	0.13
(1,2468)	1:101:A:LYS:HB2	1:103:A:ALA:H	8	0.13
(1,2416)	1:99:A:ILE:HD11	1:104:A:ALA:H	2	0.13
(1,2416)	1:99:A:ILE:HD12	1:104:A:ALA:H	2	0.13
(1,2416)	1:99:A:ILE:HD13	1:104:A:ALA:H	2	0.13
(1,2415)	1:99:A:ILE:HD11	1:103:A:ALA:H	7	0.13
(1,2415)	1:99:A:ILE:HD12	1:103:A:ALA:H	7	0.13
(1,2415)	1:99:A:ILE:HD13	1:103:A:ALA:H	7	0.13
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG21	6	0.13
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG22	6	0.13
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG23	6	0.13
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB1	6	0.13
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB2	6	0.13
(1,2232)	1:91:A:ASN:HB3	1:94:A:ALA:HB3	6	0.13
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	2	0.13
(1,1963)	1:77:A:VAL:HG21	1:77:A:VAL:HA	4	0.13
(1,1963)	1:77:A:VAL:HG22	1:77:A:VAL:HA	4	0.13
(1,1963)	1:77:A:VAL:HG23	1:77:A:VAL:HA	4	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	2	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	2	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	2	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	2	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	2	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	2	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	2	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	2	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	2	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	3	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	3	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	3	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	3	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	3	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	3	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	3	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	3	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	3	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	7	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	7	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	7	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	7	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	7	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	7	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	7	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	7	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	7	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	8	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	8	0.13
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	8	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	8	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	8	0.13
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	8	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	8	0.13
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	8	0.13
(1,1740)	1:69:A:ILE:HD11	1:69:A:ILE:HG12	8	0.13
(1,1740)	1:69:A:ILE:HD12	1:69:A:ILE:HG12	8	0.13
(1,1740)	1:69:A:ILE:HD13	1:69:A:ILE:HG12	8	0.13
(1,1739)	1:69:A:ILE:HD11	1:69:A:ILE:HG13	7	0.13
(1,1739)	1:69:A:ILE:HD12	1:69:A:ILE:HG13	7	0.13
(1,1739)	1:69:A:ILE:HD13	1:69:A:ILE:HG13	7	0.13
(1,1739)	1:69:A:ILE:HD11	1:69:A:ILE:HG13	8	0.13
(1,1739)	1:69:A:ILE:HD12	1:69:A:ILE:HG13	8	0.13
(1,1739)	1:69:A:ILE:HD13	1:69:A:ILE:HG13	8	0.13
(1,1703)	1:67:A:GLU:H	1:68:A:ASN:HB2	5	0.13
(1,1703)	1:67:A:GLU:H	1:68:A:ASN:HB2	6	0.13
(1,1607)	1:62:A:GLU:HB3	1:63:A:VAL:H	7	0.13
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG21	6	0.13
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG22	6	0.13
(1,1556)	1:57:A:VAL:H	1:57:A:VAL:HG23	6	0.13
(1,1505)	1:54:A:LYS:HA	1:54:A:LYS:HG3	6	0.13
(1,1488)	1:52:A:PHE:HZ	1:99:A:ILE:HG12	8	0.13
(1,1448)	1:51:A:VAL:HG11	1:51:A:VAL:HA	10	0.13
(1,1448)	1:51:A:VAL:HG12	1:51:A:VAL:HA	10	0.13
(1,1448)	1:51:A:VAL:HG13	1:51:A:VAL:HA	10	0.13
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD2	2	0.13
(1,1421)	1:49:A:LYS:H	1:49:A:LYS:HD3	2	0.13
(1,1218)	1:40:A:TYR:H	1:92:A:ASP:HA	7	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	1	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	2	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	3	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	4	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	5	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	6	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	7	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	8	0.13
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	10	0.13
(1,1084)	1:36:A:ILE:HG21	1:40:A:TYR:HB2	7	0.13
(1,1084)	1:36:A:ILE:HG22	1:40:A:TYR:HB2	7	0.13
(1,1084)	1:36:A:ILE:HG23	1:40:A:TYR:HB2	7	0.13
(1,1079)	1:36:A:ILE:HG21	1:37:A:ALA:H	8	0.13
(1,1079)	1:36:A:ILE:HG22	1:37:A:ALA:H	8	0.13
(1,1079)	1:36:A:ILE:HG23	1:37:A:ALA:H	8	0.13
(1,1075)	1:36:A:ILE:HG12	1:75:A:PHE:HZ	2	0.13
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	9	0.13
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB1	5	0.13
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB2	5	0.13
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB3	5	0.13
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	2	0.13
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	3	0.13
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	5	0.13
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	8	0.13
(1,780)	1:24:A:ASP:HB3	1:26:A:PHE:H	1	0.13
(1,780)	1:24:A:ASP:HB3	1:26:A:PHE:H	2	0.13
(1,780)	1:24:A:ASP:HB3	1:26:A:PHE:H	7	0.13
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	10	0.13
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	10	0.13
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	10	0.13
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	2	0.13
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	2	0.13
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	2	0.13
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	2	0.13
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	2	0.13
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	2	0.13
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	2	0.13
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	2	0.13
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	2	0.13
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	2	0.13
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	3	0.13
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	8	0.13
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	9	0.13
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	10	0.13
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	2	0.13
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	8	0.13
(1,577)	1:20:A:LEU:HD11	1:79:A:LYS:HA	8	0.13
(1,577)	1:20:A:LEU:HD12	1:79:A:LYS:HA	8	0.13
(1,577)	1:20:A:LEU:HD13	1:79:A:LYS:HA	8	0.13
(1,460)	1:17:A:GLN:HA	1:17:A:GLN:HG2	3	0.13
(1,433)	1:15:A:ILE:HG21	1:82:A:SER:HA	4	0.13
(1,433)	1:15:A:ILE:HG22	1:82:A:SER:HA	4	0.13
(1,433)	1:15:A:ILE:HG23	1:82:A:SER:HA	4	0.13
(1,433)	1:15:A:ILE:HG21	1:82:A:SER:HA	7	0.13
(1,433)	1:15:A:ILE:HG22	1:82:A:SER:HA	7	0.13
(1,433)	1:15:A:ILE:HG23	1:82:A:SER:HA	7	0.13
(1,401)	1:15:A:ILE:HG13	1:21:A:VAL:HB	6	0.13
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	3	0.13
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	10	0.13
(1,43)	1:3:A:LYS:HG3	1:4:A:ILE:H	3	0.13
(1,43)	1:3:A:LYS:HG3	1:4:A:ILE:H	10	0.13
(2,377)	1:78:A:TYR:H	1:83:A:SER:HA	6	0.12
(2,373)	1:77:A:VAL:H	1:83:A:SER:HA	7	0.12
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE1	4	0.12
(2,372)	1:77:A:VAL:HA	1:78:A:TYR:HE2	4	0.12
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	1	0.12
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	1	0.12
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	1	0.12
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	5	0.12
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	5	0.12
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	5	0.12
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	10	0.12
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	10	0.12
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	10	0.12
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	6	0.12
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	6	0.12
(2,206)	1:40:A:TYR:HD1	1:41:A:GLU:HA	9	0.12
(2,206)	1:40:A:TYR:HD2	1:41:A:GLU:HA	9	0.12
(2,197)	1:36:A:ILE:HA	1:92:A:ASP:H	7	0.12
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	4	0.12
(2,90)	1:14:A:ILE:H	1:17:A:GLN:H	7	0.12
(2,89)	1:14:A:ILE:H	1:17:A:GLN:HB2	10	0.12
(1,2549)	1:27:A:ALA:HB1	1:30:A:CYS:HB3	6	0.12
(1,2549)	1:27:A:ALA:HB2	1:30:A:CYS:HB3	6	0.12
(1,2549)	1:27:A:ALA:HB3	1:30:A:CYS:HB3	6	0.12
(1,2542)	1:26:A:PHE:HE1	1:55:A:VAL:HA	6	0.12
(1,2542)	1:26:A:PHE:HE2	1:55:A:VAL:HA	6	0.12
(1,2535)	1:103:A:ALA:H	1:104:A:ALA:HA	9	0.12
(1,2506)	1:101:A:LYS:H	1:103:A:ALA:H	3	0.12
(1,2468)	1:101:A:LYS:HB2	1:103:A:ALA:H	7	0.12
(1,2415)	1:99:A:ILE:HD11	1:103:A:ALA:H	5	0.12
(1,2415)	1:99:A:ILE:HD12	1:103:A:ALA:H	5	0.12
(1,2415)	1:99:A:ILE:HD13	1:103:A:ALA:H	5	0.12
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG21	4	0.12
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG22	4	0.12
(1,2324)	1:96:A:LYS:HA	1:99:A:ILE:HG23	4	0.12
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	6	0.12
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB1	8	0.12
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB2	8	0.12
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2197)	1:88:A:LEU:HD11	1:89:A:GLY:H	1	0.12
(1,2197)	1:88:A:LEU:HD12	1:89:A:GLY:H	1	0.12
(1,2197)	1:88:A:LEU:HD13	1:89:A:GLY:H	1	0.12
(1,2197)	1:88:A:LEU:HD21	1:89:A:GLY:H	1	0.12
(1,2197)	1:88:A:LEU:HD22	1:89:A:GLY:H	1	0.12
(1,2197)	1:88:A:LEU:HD23	1:89:A:GLY:H	1	0.12
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB1	3	0.12
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB2	3	0.12
(1,2173)	1:87:A:LEU:HD11	1:94:A:ALA:HB3	3	0.12
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB1	3	0.12
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB2	3	0.12
(1,2173)	1:87:A:LEU:HD12	1:94:A:ALA:HB3	3	0.12
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB1	3	0.12
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB2	3	0.12
(1,2173)	1:87:A:LEU:HD13	1:94:A:ALA:HB3	3	0.12
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	4	0.12
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	8	0.12
(1,1988)	1:77:A:VAL:H	1:84:A:VAL:HB	2	0.12
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	6	0.12
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	6	0.12
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	6	0.12
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	6	0.12
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	6	0.12
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	6	0.12
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	6	0.12
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	6	0.12
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	6	0.12
(1,1931)	1:77:A:VAL:HB	1:83:A:SER:HB3	6	0.12
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG21	5	0.12
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG22	5	0.12
(1,1918)	1:76:A:LYS:HE2	1:86:A:THR:HG23	5	0.12
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG21	10	0.12
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG22	10	0.12
(1,1741)	1:69:A:ILE:HD11	1:69:A:ILE:HG23	10	0.12
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG21	10	0.12
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG22	10	0.12
(1,1741)	1:69:A:ILE:HD12	1:69:A:ILE:HG23	10	0.12
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG21	10	0.12
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG22	10	0.12
(1,1741)	1:69:A:ILE:HD13	1:69:A:ILE:HG23	10	0.12
(1,1740)	1:69:A:ILE:HD11	1:69:A:ILE:HG12	3	0.12
(1,1740)	1:69:A:ILE:HD12	1:69:A:ILE:HG12	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1740)	1:69:A:ILE:HD13	1:69:A:ILE:HG12	3	0.12
(1,1740)	1:69:A:ILE:HD11	1:69:A:ILE:HG12	7	0.12
(1,1740)	1:69:A:ILE:HD12	1:69:A:ILE:HG12	7	0.12
(1,1740)	1:69:A:ILE:HD13	1:69:A:ILE:HG12	7	0.12
(1,1739)	1:69:A:ILE:HD11	1:69:A:ILE:HG13	3	0.12
(1,1739)	1:69:A:ILE:HD12	1:69:A:ILE:HG13	3	0.12
(1,1739)	1:69:A:ILE:HD13	1:69:A:ILE:HG13	3	0.12
(1,1737)	1:69:A:ILE:HD11	1:69:A:ILE:HA	3	0.12
(1,1737)	1:69:A:ILE:HD12	1:69:A:ILE:HA	3	0.12
(1,1737)	1:69:A:ILE:HD13	1:69:A:ILE:HA	3	0.12
(1,1703)	1:67:A:GLU:H	1:68:A:ASN:HB2	10	0.12
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	3	0.12
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	3	0.12
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	3	0.12
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	4	0.12
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	4	0.12
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	4	0.12
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	5	0.12
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	5	0.12
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	5	0.12
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	7	0.12
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	7	0.12
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	7	0.12
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	9	0.12
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	9	0.12
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	9	0.12
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	10	0.12
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	10	0.12
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	10	0.12
(1,1505)	1:54:A:LYS:HA	1:54:A:LYS:HG3	1	0.12
(1,1433)	1:50:A:MET:HG3	1:103:A:ALA:H	3	0.12
(1,1200)	1:40:A:TYR:HB2	1:40:A:TYR:HB3	9	0.12
(1,1133)	1:39:A:PHE:HB2	1:41:A:GLU:H	1	0.12
(1,1075)	1:36:A:ILE:HG12	1:75:A:PHE:HZ	4	0.12
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	7	0.12
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	7	0.12
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB1	3	0.12
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB2	3	0.12
(1,990)	1:33:A:CYS:HA	1:90:A:ALA:HB3	3	0.12
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	4	0.12
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	7	0.12
(1,788)	1:24:A:ASP:HB2	1:75:A:PHE:HE1	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,788)	1:24:A:ASP:HB2	1:75:A:PHE:HE2	1	0.12
(1,780)	1:24:A:ASP:HB3	1:26:A:PHE:H	9	0.12
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	4	0.12
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	4	0.12
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	4	0.12
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	3	0.12
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	3	0.12
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	3	0.12
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	3	0.12
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	3	0.12
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	3	0.12
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	3	0.12
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	3	0.12
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	3	0.12
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	7	0.12
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	7	0.12
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	7	0.12
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	7	0.12
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	7	0.12
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	7	0.12
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	7	0.12
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	7	0.12
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	7	0.12
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	5	0.12
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	2	0.12
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	1	0.12
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	4	0.12
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	2	0.12
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	5	0.12
(1,460)	1:17:A:GLN:HA	1:17:A:GLN:HG2	4	0.12
(1,460)	1:17:A:GLN:HA	1:17:A:GLN:HG2	9	0.12
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	6	0.12
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	8	0.12
(1,433)	1:15:A:ILE:HG21	1:82:A:SER:HA	8	0.12
(1,433)	1:15:A:ILE:HG22	1:82:A:SER:HA	8	0.12
(1,433)	1:15:A:ILE:HG23	1:82:A:SER:HA	8	0.12
(1,433)	1:15:A:ILE:HG21	1:82:A:SER:HA	10	0.12
(1,433)	1:15:A:ILE:HG22	1:82:A:SER:HA	10	0.12
(1,433)	1:15:A:ILE:HG23	1:82:A:SER:HA	10	0.12
(1,401)	1:15:A:ILE:HG13	1:21:A:VAL:HB	7	0.12
(1,401)	1:15:A:ILE:HG13	1:21:A:VAL:HB	9	0.12
(1,400)	1:15:A:ILE:HG13	1:17:A:GLN:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:15:A:ILE:HD11	1:23:A:VAL:HB	10	0.12
(1,380)	1:15:A:ILE:HD12	1:23:A:VAL:HB	10	0.12
(1,380)	1:15:A:ILE:HD13	1:23:A:VAL:HB	10	0.12
(1,194)	1:10:A:GLU:H	1:10:A:GLU:HG2	9	0.12
(1,194)	1:10:A:GLU:H	1:10:A:GLU:HG3	9	0.12
(1,164)	1:8:A:GLN:H	1:8:A:GLN:HG2	9	0.12
(1,164)	1:8:A:GLN:H	1:8:A:GLN:HG2	10	0.12
(1,105)	1:5:A:VAL:H	1:55:A:VAL:HB	9	0.12
(1,54)	1:3:A:LYS:H	1:3:A:LYS:HG2	2	0.12
(1,54)	1:3:A:LYS:H	1:3:A:LYS:HG2	5	0.12
(1,44)	1:3:A:LYS:HG3	1:53:A:ILE:HA	10	0.12
(1,12)	1:2:A:VAL:HG11	1:3:A:LYS:H	7	0.12
(1,12)	1:2:A:VAL:HG12	1:3:A:LYS:H	7	0.12
(1,12)	1:2:A:VAL:HG13	1:3:A:LYS:H	7	0.12
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE1	1	0.11
(2,359)	1:74:A:THR:H	1:75:A:PHE:HE2	1	0.11
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD11	7	0.11
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD12	7	0.11
(2,303)	1:68:A:ASN:HD21	1:69:A:ILE:HD13	7	0.11
(2,287)	1:57:A:VAL:HG21	1:61:A:SER:HA	6	0.11
(2,287)	1:57:A:VAL:HG22	1:61:A:SER:HA	6	0.11
(2,287)	1:57:A:VAL:HG23	1:61:A:SER:HA	6	0.11
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE1	7	0.11
(2,268)	1:51:A:VAL:H	1:52:A:PHE:HE2	7	0.11
(2,242)	1:47:A:TYR:HA	1:50:A:MET:HB3	5	0.11
(2,229)	1:44:A:SER:HG	1:45:A:LYS:HD2	7	0.11
(2,229)	1:44:A:SER:HG	1:45:A:LYS:HD3	7	0.11
(2,166)	1:28:A:GLU:H	1:29:A:TRP:HE1	3	0.11
(2,166)	1:28:A:GLU:H	1:29:A:TRP:HE1	6	0.11
(2,166)	1:28:A:GLU:H	1:29:A:TRP:HE1	7	0.11
(2,166)	1:28:A:GLU:H	1:29:A:TRP:HE1	8	0.11
(2,166)	1:28:A:GLU:H	1:29:A:TRP:HE1	10	0.11
(2,114)	1:24:A:ASP:H	1:25:A:PHE:HA	1	0.11
(2,91)	1:15:A:ILE:HA	1:18:A:ASN:H	9	0.11
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE2	4	0.11
(2,83)	1:12:A:ASP:HB2	1:66:A:LYS:HE3	4	0.11
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE2	4	0.11
(2,80)	1:12:A:ASP:HB3	1:66:A:LYS:HE3	4	0.11
(2,19)	1:2:A:VAL:HB	1:3:A:LYS:HA	2	0.11
(1,2542)	1:26:A:PHE:HE1	1:55:A:VAL:HA	3	0.11
(1,2542)	1:26:A:PHE:HE2	1:55:A:VAL:HA	3	0.11
(1,2506)	1:101:A:LYS:H	1:103:A:ALA:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2465)	1:101:A:LYS:HB3	1:103:A:ALA:H	1	0.11
(1,2463)	1:101:A:LYS:HA	1:104:A:ALA:H	2	0.11
(1,2463)	1:101:A:LYS:HA	1:104:A:ALA:H	7	0.11
(1,2409)	1:99:A:ILE:HD11	1:99:A:ILE:HA	1	0.11
(1,2409)	1:99:A:ILE:HD12	1:99:A:ILE:HA	1	0.11
(1,2409)	1:99:A:ILE:HD13	1:99:A:ILE:HA	1	0.11
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	1	0.11
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	3	0.11
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	4	0.11
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	7	0.11
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB1	3	0.11
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB2	3	0.11
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB3	3	0.11
(1,2200)	1:88:A:LEU:HD21	1:88:A:LEU:HA	7	0.11
(1,2200)	1:88:A:LEU:HD22	1:88:A:LEU:HA	7	0.11
(1,2200)	1:88:A:LEU:HD23	1:88:A:LEU:HA	7	0.11
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	1	0.11
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	3	0.11
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	5	0.11
(1,2156)	1:86:A:THR:H	1:86:A:THR:HB	10	0.11
(1,1988)	1:77:A:VAL:H	1:84:A:VAL:HB	9	0.11
(1,1988)	1:77:A:VAL:H	1:84:A:VAL:HB	10	0.11
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG21	5	0.11
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG22	5	0.11
(1,1940)	1:77:A:VAL:HG11	1:77:A:VAL:HG23	5	0.11
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG21	5	0.11
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG22	5	0.11
(1,1940)	1:77:A:VAL:HG12	1:77:A:VAL:HG23	5	0.11
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG21	5	0.11
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG22	5	0.11
(1,1940)	1:77:A:VAL:HG13	1:77:A:VAL:HG23	5	0.11
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	3	0.11
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	3	0.11
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	3	0.11
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG21	10	0.11
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG22	10	0.11
(1,1812)	1:74:A:THR:HG1	1:74:A:THR:HG23	10	0.11
(1,1739)	1:69:A:ILE:HD11	1:69:A:ILE:HG13	2	0.11
(1,1739)	1:69:A:ILE:HD12	1:69:A:ILE:HG13	2	0.11
(1,1739)	1:69:A:ILE:HD13	1:69:A:ILE:HG13	2	0.11
(1,1666)	1:64:A:THR:HG21	1:69:A:ILE:H	7	0.11
(1,1666)	1:64:A:THR:HG22	1:69:A:ILE:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1666)	1:64:A:THR:HG23	1:69:A:ILE:H	7	0.11
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	1	0.11
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	1	0.11
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	1	0.11
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	2	0.11
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	2	0.11
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	2	0.11
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	6	0.11
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	6	0.11
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	6	0.11
(1,1625)	1:63:A:VAL:HG11	1:63:A:VAL:HB	8	0.11
(1,1625)	1:63:A:VAL:HG12	1:63:A:VAL:HB	8	0.11
(1,1625)	1:63:A:VAL:HG13	1:63:A:VAL:HB	8	0.11
(1,1550)	1:57:A:VAL:HG21	1:58:A:ASP:H	10	0.11
(1,1550)	1:57:A:VAL:HG22	1:58:A:ASP:H	10	0.11
(1,1550)	1:57:A:VAL:HG23	1:58:A:ASP:H	10	0.11
(1,1505)	1:54:A:LYS:HA	1:54:A:LYS:HG3	4	0.11
(1,1486)	1:52:A:PHE:HZ	1:99:A:ILE:HA	10	0.11
(1,1432)	1:50:A:MET:HG3	1:52:A:PHE:HZ	7	0.11
(1,1432)	1:50:A:MET:HG3	1:52:A:PHE:HZ	8	0.11
(1,1259)	1:43:A:CYS:HA	1:52:A:PHE:HZ	7	0.11
(1,1259)	1:43:A:CYS:HA	1:52:A:PHE:HZ	8	0.11
(1,1218)	1:40:A:TYR:H	1:92:A:ASP:HA	8	0.11
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD21	8	0.11
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD22	8	0.11
(1,1207)	1:40:A:TYR:HD1	1:95:A:LEU:HD23	8	0.11
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD21	8	0.11
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD22	8	0.11
(1,1207)	1:40:A:TYR:HD2	1:95:A:LEU:HD23	8	0.11
(1,1133)	1:39:A:PHE:HB2	1:41:A:GLU:H	9	0.11
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	7	0.11
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	7	0.11
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD2	10	0.11
(1,1100)	1:36:A:ILE:H	1:38:A:PRO:HD3	10	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB1	5	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB2	5	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB3	5	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB1	5	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB2	5	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB3	5	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB1	5	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB3	5	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB1	7	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB2	7	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB3	7	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB1	7	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB2	7	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB3	7	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB1	7	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB2	7	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB3	7	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB1	8	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB2	8	0.11
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB3	8	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB1	8	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB2	8	0.11
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB3	8	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB1	8	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB2	8	0.11
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB3	8	0.11
(1,1088)	1:36:A:ILE:HG21	1:75:A:PHE:HZ	1	0.11
(1,1088)	1:36:A:ILE:HG22	1:75:A:PHE:HZ	1	0.11
(1,1088)	1:36:A:ILE:HG23	1:75:A:PHE:HZ	1	0.11
(1,1077)	1:36:A:ILE:HG21	1:36:A:ILE:HG13	3	0.11
(1,1077)	1:36:A:ILE:HG22	1:36:A:ILE:HG13	3	0.11
(1,1077)	1:36:A:ILE:HG23	1:36:A:ILE:HG13	3	0.11
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE1	10	0.11
(1,1074)	1:36:A:ILE:HG12	1:75:A:PHE:HE2	10	0.11
(1,1051)	1:36:A:ILE:HA	1:92:A:ASP:HA	3	0.11
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	10	0.11
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	10	0.11
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	10	0.11
(1,975)	1:32:A:PRO:HA	1:36:A:ILE:HA	1	0.11
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE1	9	0.11
(1,731)	1:23:A:VAL:HG11	1:78:A:TYR:HE2	9	0.11
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE1	9	0.11
(1,731)	1:23:A:VAL:HG12	1:78:A:TYR:HE2	9	0.11
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE1	9	0.11
(1,731)	1:23:A:VAL:HG13	1:78:A:TYR:HE2	9	0.11
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	4	0.11
(1,688)	1:22:A:ILE:H	1:50:A:MET:HA	2	0.11
(1,654)	1:22:A:ILE:HD11	1:75:A:PHE:HB3	9	0.11
(1,654)	1:22:A:ILE:HD12	1:75:A:PHE:HB3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:22:A:ILE:HD13	1:75:A:PHE:HB3	9	0.11
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	1	0.11
(1,612)	1:21:A:VAL:HB	1:78:A:TYR:HB2	7	0.11
(1,594)	1:20:A:LEU:H	1:50:A:MET:HA	5	0.11
(1,586)	1:20:A:LEU:HG	1:51:A:VAL:H	3	0.11
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	3	0.11
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	4	0.11
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	6	0.11
(1,524)	1:19:A:GLU:HA	1:79:A:LYS:HA	8	0.11
(1,460)	1:17:A:GLN:HA	1:17:A:GLN:HG2	10	0.11
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	3	0.11
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	4	0.11
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	5	0.11
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	9	0.11
(1,431)	1:15:A:ILE:HG21	1:81:A:GLY:HA2	7	0.11
(1,431)	1:15:A:ILE:HG22	1:81:A:GLY:HA2	7	0.11
(1,431)	1:15:A:ILE:HG23	1:81:A:GLY:HA2	7	0.11
(1,401)	1:15:A:ILE:HG13	1:21:A:VAL:HB	2	0.11
(1,401)	1:15:A:ILE:HG13	1:21:A:VAL:HB	3	0.11
(1,223)	1:11:A:PHE:HE1	1:15:A:ILE:HD11	3	0.11
(1,223)	1:11:A:PHE:HE1	1:15:A:ILE:HD12	3	0.11
(1,223)	1:11:A:PHE:HE1	1:15:A:ILE:HD13	3	0.11
(1,223)	1:11:A:PHE:HE2	1:15:A:ILE:HD11	3	0.11
(1,223)	1:11:A:PHE:HE2	1:15:A:ILE:HD12	3	0.11
(1,223)	1:11:A:PHE:HE2	1:15:A:ILE:HD13	3	0.11
(1,105)	1:5:A:VAL:H	1:55:A:VAL:HB	3	0.11
(1,83)	1:5:A:VAL:HG11	1:11:A:PHE:HA	10	0.11
(1,83)	1:5:A:VAL:HG12	1:11:A:PHE:HA	10	0.11
(1,83)	1:5:A:VAL:HG13	1:11:A:PHE:HA	10	0.11
(1,54)	1:3:A:LYS:H	1:3:A:LYS:HG2	8	0.11
(1,47)	1:3:A:LYS:HG2	1:53:A:ILE:HA	3	0.11
(1,44)	1:3:A:LYS:HG3	1:53:A:ILE:HA	1	0.11
(1,43)	1:3:A:LYS:HG3	1:4:A:ILE:H	1	0.11
(1,43)	1:3:A:LYS:HG3	1:4:A:ILE:H	6	0.11
(1,8)	1:2:A:VAL:HA	1:53:A:ILE:H	4	0.11
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD1	10	0.1
(2,247)	1:47:A:TYR:HB2	1:52:A:PHE:HD2	10	0.1
(2,197)	1:36:A:ILE:HA	1:92:A:ASP:H	2	0.1
(2,197)	1:36:A:ILE:HA	1:92:A:ASP:H	9	0.1
(2,143)	1:26:A:PHE:H	1:56:A:ASP:HB2	8	0.1
(2,89)	1:14:A:ILE:H	1:17:A:GLN:HB2	9	0.1
(2,19)	1:2:A:VAL:HB	1:3:A:LYS:HA	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2534)	1:103:A:ALA:H	1:103:A:ALA:HB1	5	0.1
(1,2534)	1:103:A:ALA:H	1:103:A:ALA:HB2	5	0.1
(1,2534)	1:103:A:ALA:H	1:103:A:ALA:HB3	5	0.1
(1,2468)	1:101:A:LYS:HB2	1:103:A:ALA:H	1	0.1
(1,2468)	1:101:A:LYS:HB2	1:103:A:ALA:H	9	0.1
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	5	0.1
(1,2289)	1:94:A:ALA:HA	1:98:A:LEU:H	10	0.1
(1,2275)	1:93:A:SER:HB2	1:96:A:LYS:H	6	0.1
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB1	6	0.1
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB2	6	0.1
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB3	6	0.1
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB1	9	0.1
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB2	9	0.1
(1,2225)	1:90:A:ALA:H	1:90:A:ALA:HB3	9	0.1
(1,1958)	1:77:A:VAL:HG11	1:102:A:TYR:HB3	7	0.1
(1,1958)	1:77:A:VAL:HG12	1:102:A:TYR:HB3	7	0.1
(1,1958)	1:77:A:VAL:HG13	1:102:A:TYR:HB3	7	0.1
(1,1740)	1:69:A:ILE:HD11	1:69:A:ILE:HG12	2	0.1
(1,1740)	1:69:A:ILE:HD12	1:69:A:ILE:HG12	2	0.1
(1,1740)	1:69:A:ILE:HD13	1:69:A:ILE:HG12	2	0.1
(1,1486)	1:52:A:PHE:HZ	1:99:A:ILE:HA	2	0.1
(1,1378)	1:47:A:TYR:HD1	1:99:A:ILE:HG21	9	0.1
(1,1378)	1:47:A:TYR:HD1	1:99:A:ILE:HG22	9	0.1
(1,1378)	1:47:A:TYR:HD1	1:99:A:ILE:HG23	9	0.1
(1,1378)	1:47:A:TYR:HD2	1:99:A:ILE:HG21	9	0.1
(1,1378)	1:47:A:TYR:HD2	1:99:A:ILE:HG22	9	0.1
(1,1378)	1:47:A:TYR:HD2	1:99:A:ILE:HG23	9	0.1
(1,1377)	1:47:A:TYR:HD1	1:99:A:ILE:HG21	9	0.1
(1,1377)	1:47:A:TYR:HD1	1:99:A:ILE:HG22	9	0.1
(1,1377)	1:47:A:TYR:HD1	1:99:A:ILE:HG23	9	0.1
(1,1377)	1:47:A:TYR:HD2	1:99:A:ILE:HG21	9	0.1
(1,1377)	1:47:A:TYR:HD2	1:99:A:ILE:HG22	9	0.1
(1,1377)	1:47:A:TYR:HD2	1:99:A:ILE:HG23	9	0.1
(1,1321)	1:45:A:LYS:H	1:45:A:LYS:HG3	10	0.1
(1,1316)	1:45:A:LYS:HG3	1:46:A:THR:H	10	0.1
(1,1218)	1:40:A:TYR:H	1:92:A:ASP:HA	9	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB1	2	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB2	2	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB3	2	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB1	2	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB2	2	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB3	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB1	2	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB2	2	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB3	2	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB1	3	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB2	3	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB3	3	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB1	3	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB2	3	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB3	3	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB1	3	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB2	3	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB3	3	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB1	4	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB2	4	0.1
(1,1090)	1:36:A:ILE:HG21	1:90:A:ALA:HB3	4	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB1	4	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB2	4	0.1
(1,1090)	1:36:A:ILE:HG22	1:90:A:ALA:HB3	4	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB1	4	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB2	4	0.1
(1,1090)	1:36:A:ILE:HG23	1:90:A:ALA:HB3	4	0.1
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG21	7	0.1
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG22	7	0.1
(1,989)	1:33:A:CYS:HA	1:36:A:ILE:HG23	7	0.1
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB1	2	0.1
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB2	2	0.1
(1,985)	1:32:A:PRO:HB2	1:90:A:ALA:HB3	2	0.1
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG11	8	0.1
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG12	8	0.1
(1,764)	1:23:A:VAL:H	1:23:A:VAL:HG13	8	0.1
(1,753)	1:23:A:VAL:HG21	1:55:A:VAL:H	10	0.1
(1,753)	1:23:A:VAL:HG22	1:55:A:VAL:H	10	0.1
(1,753)	1:23:A:VAL:HG23	1:55:A:VAL:H	10	0.1
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG11	5	0.1
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG12	5	0.1
(1,735)	1:23:A:VAL:HG21	1:23:A:VAL:HG13	5	0.1
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG11	5	0.1
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG12	5	0.1
(1,735)	1:23:A:VAL:HG22	1:23:A:VAL:HG13	5	0.1
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG11	5	0.1
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG12	5	0.1
(1,735)	1:23:A:VAL:HG23	1:23:A:VAL:HG13	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:23:A:VAL:HG11	1:25:A:PHE:HE1	9	0.1
(1,710)	1:23:A:VAL:HG11	1:25:A:PHE:HE2	9	0.1
(1,710)	1:23:A:VAL:HG12	1:25:A:PHE:HE1	9	0.1
(1,710)	1:23:A:VAL:HG12	1:25:A:PHE:HE2	9	0.1
(1,710)	1:23:A:VAL:HG13	1:25:A:PHE:HE1	9	0.1
(1,710)	1:23:A:VAL:HG13	1:25:A:PHE:HE2	9	0.1
(1,697)	1:22:A:ILE:H	1:53:A:ILE:H	6	0.1
(1,586)	1:20:A:LEU:HG	1:51:A:VAL:H	6	0.1
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	2	0.1
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	7	0.1
(1,439)	1:15:A:ILE:H	1:15:A:ILE:HG12	10	0.1
(1,401)	1:15:A:ILE:HG13	1:21:A:VAL:HB	1	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG11	4	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG12	4	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG13	4	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG11	4	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG12	4	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG13	4	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG11	4	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG12	4	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG13	4	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG11	6	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG12	6	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG13	6	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG11	6	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG12	6	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG13	6	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG11	6	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG12	6	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG13	6	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG11	8	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG12	8	0.1
(1,375)	1:15:A:ILE:HD11	1:21:A:VAL:HG13	8	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG11	8	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG12	8	0.1
(1,375)	1:15:A:ILE:HD12	1:21:A:VAL:HG13	8	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG11	8	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG12	8	0.1
(1,375)	1:15:A:ILE:HD13	1:21:A:VAL:HG13	8	0.1
(1,322)	1:14:A:ILE:HA	1:18:A:ASN:HD21	9	0.1
(1,164)	1:8:A:GLN:H	1:8:A:GLN:HG2	2	0.1
(1,47)	1:3:A:LYS:HG2	1:53:A:ILE:HA	7	0.1

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

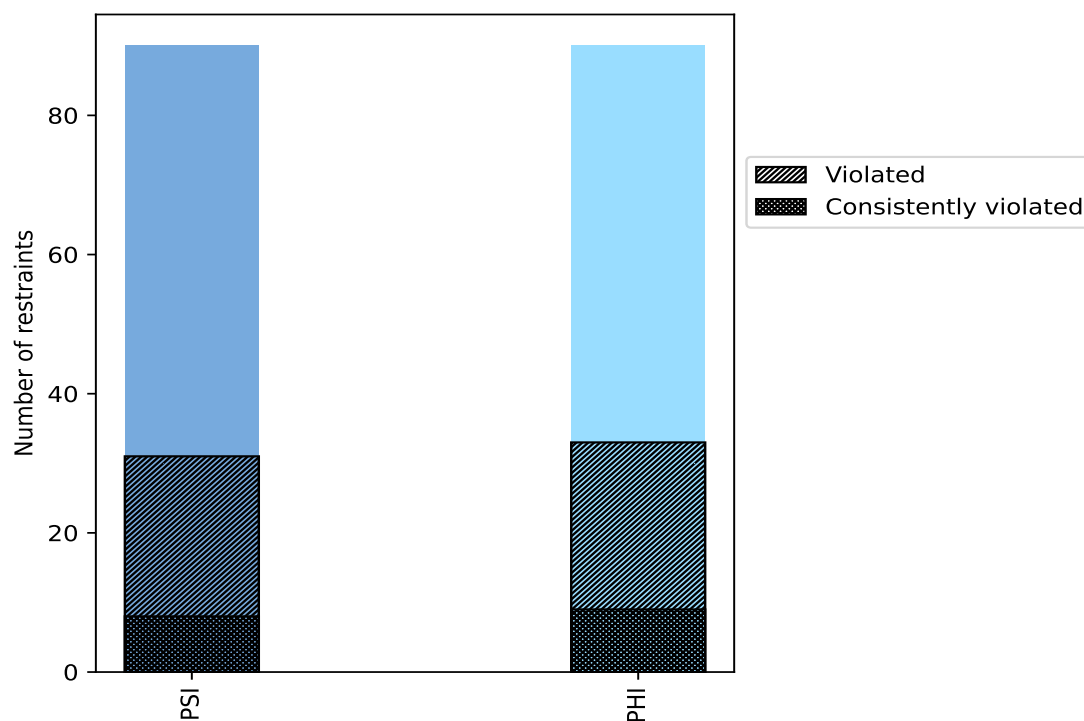
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	90	50.0	31	34.4	17.2	8	8.9	4.4
PHI	90	50.0	33	36.7	18.3	9	10.0	5.0
Total	180	100.0	64	35.6	35.6	17	9.4	9.4

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](#)



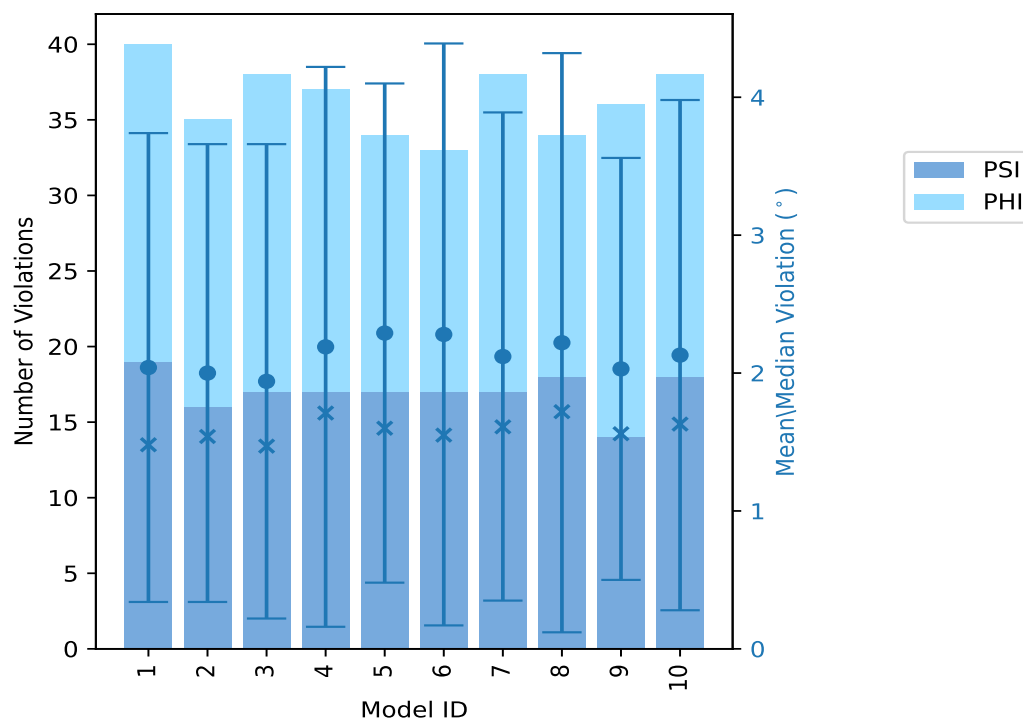
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	19	21	40	2.04	9.42	1.7	1.48
2	16	19	35	2.0	8.89	1.66	1.54
3	17	21	38	1.94	9.62	1.72	1.47
4	17	20	37	2.19	10.54	2.03	1.71
5	17	17	34	2.29	9.3	1.81	1.6
6	17	16	33	2.28	10.7	2.11	1.55
7	17	21	38	2.12	9.78	1.77	1.61
8	18	16	34	2.22	10.64	2.1	1.72
9	14	22	36	2.03	8.5	1.53	1.56
10	18	20	38	2.13	10.61	1.85	1.63

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

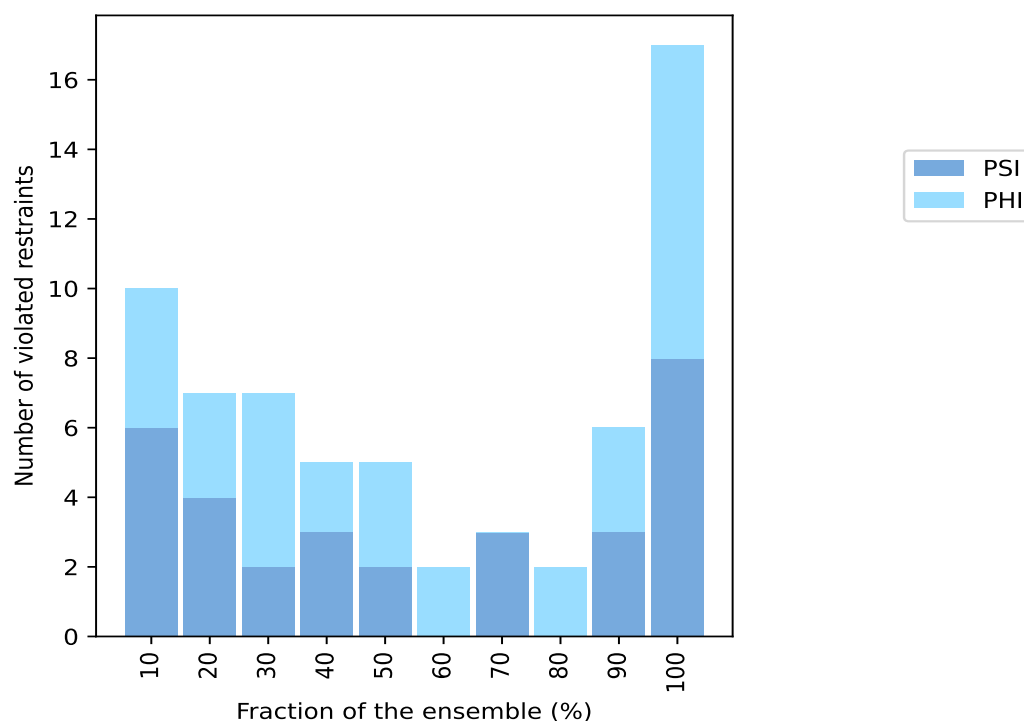
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count ¹	%
6	4	10	1	10.0
4	3	7	2	20.0
2	5	7	3	30.0
3	2	5	4	40.0
2	3	5	5	50.0
0	2	2	6	60.0
3	0	3	7	70.0
0	2	2	8	80.0
3	3	6	9	90.0
8	9	17	10	100.0

¹ Number of models with violations

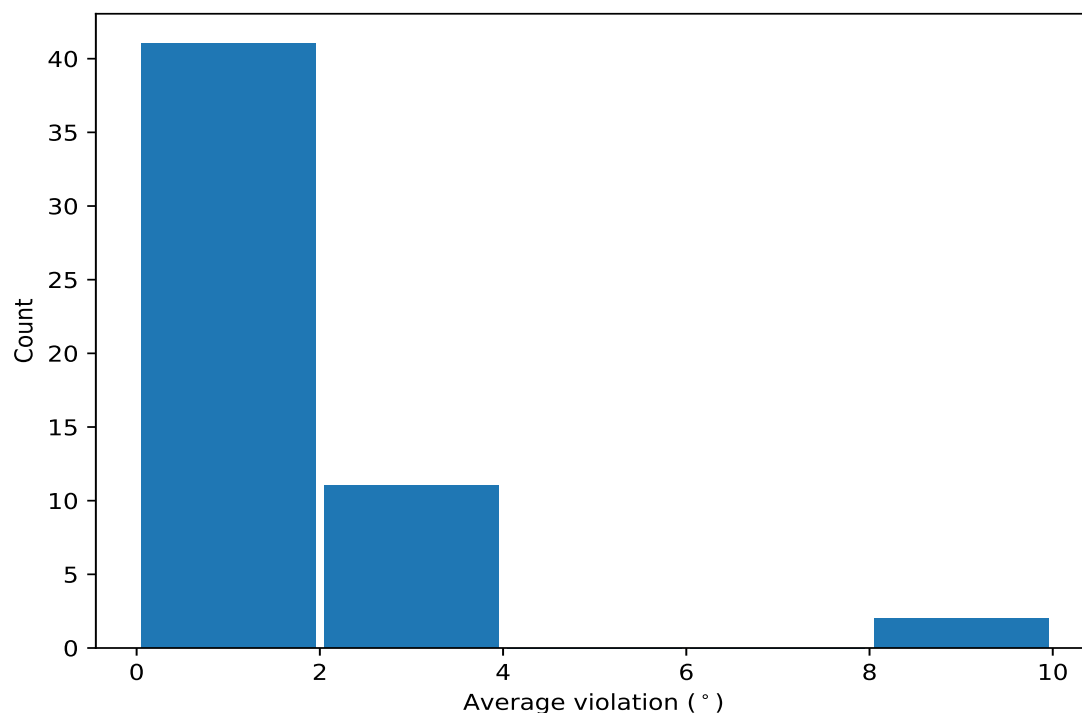
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	10	9.8	0.75	9.7
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	10	8.74	0.87	8.52
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	10	2.8	0.76	2.7
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	10	2.76	0.59	2.7
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	10	2.4	0.38	2.37
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	10	2.33	0.46	2.34
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	10	2.19	0.47	2.3
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	10	2.15	0.51	2.25
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	10	2.1	0.37	2.16
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	10	2.04	0.68	2.0
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	10	1.89	0.47	1.87
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	10	1.84	0.19	1.86
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	10	1.82	0.36	1.7

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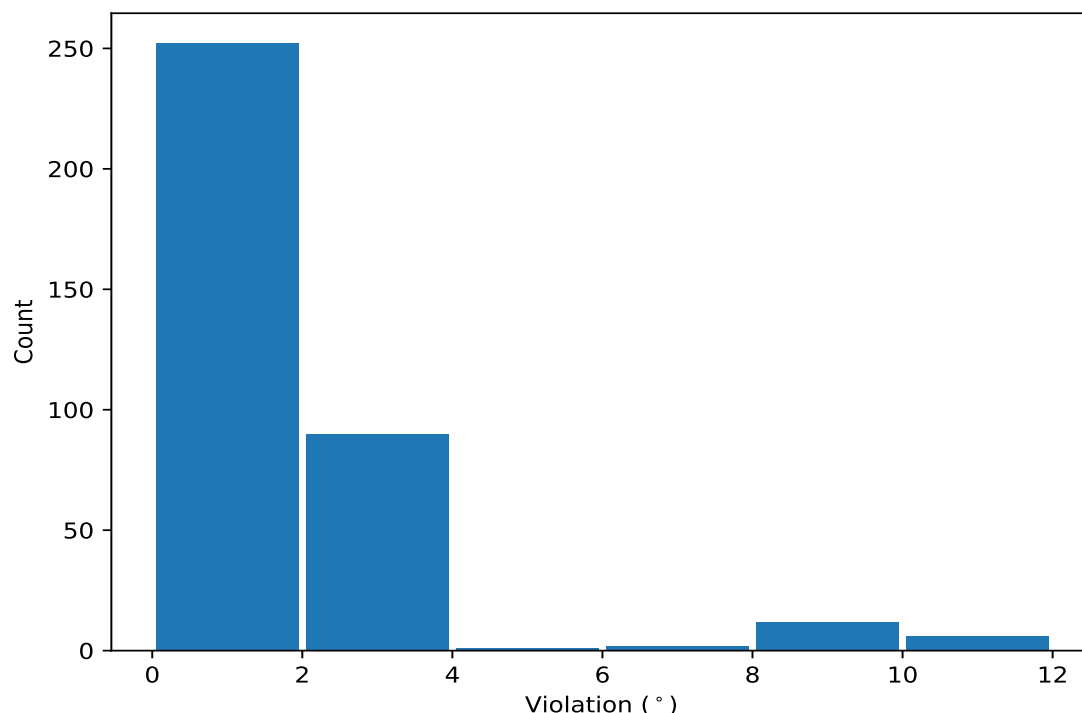
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	10	1.52	0.35	1.57
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	10	1.51	0.1	1.52
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	10	1.44	0.35	1.4
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	10	1.31	0.19	1.27
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	9	2.19	0.25	2.09
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	9	1.89	0.49	1.83
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	9	1.51	0.31	1.44
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	9	1.48	0.28	1.37
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	9	1.33	0.21	1.25
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	9	1.29	0.15	1.27
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	8	2.28	0.38	2.3
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	8	1.54	0.58	1.25
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	7	1.52	0.21	1.5
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	7	1.2	0.17	1.1
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	7	1.16	0.1	1.13
(1,175)	1:99:A:ILE:C	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	6	1.66	0.46	1.57
(1,29)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	6	1.21	0.14	1.19
(1,88)	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1:49:A:LYS:N	5	1.44	0.27	1.52
(1,2)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:ILE:N	5	1.36	0.26	1.3
(1,1)	1:2:A:VAL:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	5	1.33	0.28	1.27
(1,169)	1:96:A:LYS:C	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	5	1.32	0.27	1.24
(1,27)	1:15:A:ILE:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	5	1.14	0.09	1.08
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:VAL:N	4	1.67	0.57	1.51
(1,124)	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	1:69:A:ILE:N	4	1.4	0.19	1.32
(1,83)	1:45:A:LYS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	4	1.39	0.33	1.33
(1,24)	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	1:15:A:ILE:N	4	1.12	0.11	1.09
(1,91)	1:50:A:MET:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	4	1.06	0.03	1.06
(1,73)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	3	2.01	0.44	1.71
(1,5)	1:4:A:ILE:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	3	1.77	0.39	1.84
(1,45)	1:24:A:ASP:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	3	1.65	0.71	1.19
(1,147)	1:84:A:VAL:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	3	1.59	0.34	1.63
(1,156)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ASN:N	3	1.3	0.32	1.12
(1,139)	1:78:A:TYR:C	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	3	1.28	0.24	1.17
(1,162)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:ALA:N	3	1.23	0.11	1.22
(1,69)	1:38:A:PRO:C	1:39:A:PHE:N	1:39:A:PHE:CA	1:39:A:PHE:C	2	1.44	0.22	1.44
(1,159)	1:91:A:ASN:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	2	1.29	0.13	1.29
(1,67)	1:37:A:ALA:C	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	2	1.27	0.14	1.27
(1,100)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:ASP:N	2	1.25	0.12	1.25
(1,10)	1:7:A:SER:N	1:7:A:SER:CA	1:7:A:SER:C	1:8:A:GLN:N	2	1.14	0.13	1.14
(1,30)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:ASN:N	2	1.13	0.06	1.13
(1,78)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:SER:N	2	1.08	0.01	1.08

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	6	10.7
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	8	10.64
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	10	10.61
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	4	10.54
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	8	10.09
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	4	10.01
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	7	9.78
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	6	9.67
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	3	9.62
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	1	9.42
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	5	9.3
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	2	8.89
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	10	8.7
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	7	8.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:47:A:TYR:N	1:47:A:TYR:CA	1:47:A:TYR:C	1:48:A:THR:N	9	8.5
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	3	8.41
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1	8.35
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	5	8.34
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	2	7.8
(1,87)	1:47:A:TYR:C	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	9	7.35
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	1	4.2
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	5	3.91
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	4	3.54
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	5	3.49
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	7	3.46
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	6	3.39
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	2	3.22
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	5	3.13
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	5	3.13
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	4	3.08
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	9	3.06
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	10	3.0
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	6	2.98
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	5	2.96
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	9	2.96
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	4	2.87
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	9	2.84
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	8	2.76
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	3	2.74
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	6	2.74
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	9	2.74
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	5	2.73
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	2	2.66
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	6	2.65
(1,45)	1:24:A:ASP:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1	2.65
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	8	2.63
(1,73)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	10	2.63
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	10	2.62
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	7	2.61
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	6	2.59
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	7	2.59
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	5	2.58
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	7	2.58
(1,175)	1:99:A:ILE:C	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1	2.57
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	5	2.56
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	2	2.55
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	6	2.55
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:VAL:N	7	2.54
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	2	2.53
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	5	2.53
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	3	2.53
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	4	2.52
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	2	2.5
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	6	2.5
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	1	2.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	9	2.47
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	10	2.47
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1	2.44
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	4	2.42
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	7	2.41
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	8	2.4
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	10	2.38
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	5	2.36
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	8	2.36
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	1	2.36
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	8	2.35
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	1	2.35
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	10	2.31
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	4	2.29
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	8	2.29
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1	2.28
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	8	2.26
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	6	2.26
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	10	2.26
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	8	2.26
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	4	2.25
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	6	2.25
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	3	2.25
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	2	2.24
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	6	2.24
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	8	2.22
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	3	2.22
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	7	2.2
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	10	2.2
(1,5)	1:4:A:ILE:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	7	2.2
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	4	2.19
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	3	2.19
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	4	2.19
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	1	2.17
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	7	2.14
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	4	2.13
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	10	2.1
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	7	2.1
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	3	2.09
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	7	2.07
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	4	2.06
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	8	2.04
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	9	2.04
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	4	2.04
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	6	2.02
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	7	2.01
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	1	1.99
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	7	1.99
(1,147)	1:84:A:VAL:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	8	1.99
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	5	1.98
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	6	1.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	1	1.94
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	8	1.94
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	5	1.93
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	10	1.92
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	10	1.92
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	2	1.92
(1,176)	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	1:101:A:LYS:N	4	1.91
(1,83)	1:45:A:LYS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	10	1.91
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1	1.9
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	8	1.9
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	1	1.89
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	9	1.87
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	3	1.87
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	2	1.87
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	6	1.85
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	8	1.85
(1,5)	1:4:A:ILE:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	9	1.84
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	9	1.83
(1,178)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:TYR:N	1	1.82
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	2	1.82
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	10	1.8
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	3	1.79
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:VAL:N	9	1.79
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	4	1.78
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	10	1.78
(1,2)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:ILE:N	3	1.78
(1,169)	1:96:A:LYS:C	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	9	1.77
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	7	1.77
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	10	1.77
(1,1)	1:2:A:VAL:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1	1.77
(1,175)	1:99:A:ILE:C	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	2	1.75
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	1	1.75
(1,156)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ASN:N	9	1.75
(1,88)	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1:49:A:LYS:N	4	1.75
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	2	1.75
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	4	1.74
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	1	1.73
(1,145)	1:82:A:SER:C	1:83:A:SER:N	1:83:A:SER:CA	1:83:A:SER:C	8	1.73
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	9	1.73
(1,124)	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	1:69:A:ILE:N	8	1.72
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	3	1.72
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	3	1.71
(1,73)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	4	1.71
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	3	1.7
(1,73)	1:40:A:TYR:C	1:41:A:GLU:N	1:41:A:GLU:CA	1:41:A:GLU:C	5	1.7
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	9	1.69
(1,46)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:PHE:N	3	1.69
(1,173)	1:98:A:LEU:C	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	2	1.68
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	7	1.68
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	6	1.67
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	8	1.66

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:38:A:PRO:C	1:39:A:PHE:N	1:39:A:PHE:CA	1:39:A:PHE:C	10	1.66
(1,88)	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1:49:A:LYS:N	8	1.65
(1,71)	1:39:A:PHE:C	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	3	1.65
(1,175)	1:99:A:ILE:C	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	10	1.64
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	2	1.63
(1,147)	1:84:A:VAL:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	4	1.63
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	9	1.63
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	7	1.63
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	5	1.62
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	3	1.62
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	10	1.62
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	7	1.61
(1,139)	1:78:A:TYR:C	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	5	1.61
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	9	1.61
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	7	1.61
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	7	1.6
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	10	1.6
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	5	1.58
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	7	1.58
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	3	1.57
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	10	1.57
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	2	1.56
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	2	1.56
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	7	1.55
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	6	1.55
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	2	1.54
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	9	1.52
(1,88)	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1:49:A:LYS:N	5	1.52
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	10	1.52
(1,1)	1:2:A:VAL:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	6	1.52
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	10	1.51
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1	1.51
(1,59)	1:33:A:CYS:C	1:34:A:LYS:N	1:34:A:LYS:CA	1:34:A:LYS:C	6	1.51
(1,175)	1:99:A:ILE:C	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	9	1.5
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	9	1.5
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	2	1.5
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	10	1.5
(1,2)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:ILE:N	4	1.49
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	3	1.48
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	10	1.47
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	8	1.47
(1,29)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	10	1.47
(1,169)	1:96:A:LYS:C	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	7	1.46
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	2	1.46
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	3	1.46
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	7	1.46
(1,144)	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	1:83:A:SER:N	10	1.45
(1,127)	1:72:A:MET:C	1:73:A:PRO:N	1:73:A:PRO:CA	1:73:A:PRO:C	1	1.45
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	5	1.45
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	9	1.45
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	5	1.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	9	1.44
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	8	1.43
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	7	1.43
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1	1.42
(1,159)	1:91:A:ASN:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	7	1.42
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	4	1.41
(1,67)	1:37:A:ALA:C	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	9	1.41
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	3	1.4
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	2	1.39
(1,175)	1:99:A:ILE:C	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	3	1.39
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	5	1.39
(1,34)	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	1:20:A:LEU:N	5	1.39
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	9	1.38
(1,162)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:ALA:N	9	1.38
(1,100)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:ASP:N	2	1.38
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	1	1.38
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	7	1.37
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	8	1.37
(1,121)	1:66:A:LYS:C	1:67:A:GLU:N	1:67:A:GLU:CA	1:67:A:GLU:C	5	1.37
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	1	1.37
(1,143)	1:81:A:GLY:C	1:82:A:SER:N	1:82:A:SER:CA	1:82:A:SER:C	3	1.36
(1,124)	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	1:69:A:ILE:N	6	1.36
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	6	1.36
(1,83)	1:45:A:LYS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	5	1.34
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	2	1.34
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	2	1.33
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	9	1.33
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	8	1.32
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	4	1.32
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	9	1.32
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	5	1.32
(1,83)	1:45:A:LYS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	4	1.31
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	3	1.31
(1,39)	1:21:A:VAL:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	8	1.31
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	4	1.31
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	10	1.3
(1,2)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:ILE:N	6	1.3
(1,24)	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	1:15:A:ILE:N	3	1.29
(1,124)	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	1:69:A:ILE:N	5	1.28
(1,88)	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1:49:A:LYS:N	6	1.28
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	5	1.28
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	5	1.27
(1,27)	1:15:A:ILE:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	9	1.27
(1,10)	1:7:A:SER:N	1:7:A:SER:CA	1:7:A:SER:C	1:8:A:GLN:N	10	1.27
(1,1)	1:2:A:VAL:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	10	1.27
(1,5)	1:4:A:ILE:C	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	3	1.26
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	4	1.25
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	3	1.25
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	8	1.25
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	3	1.25
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	8	1.24

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,169)	1:96:A:LYS:C	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1	1.24
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	6	1.24
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	1	1.24
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	1	1.24
(1,29)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	4	1.24
(1,27)	1:15:A:ILE:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	3	1.24
(1,167)	1:95:A:LEU:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	1	1.23
(1,160)	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	1:93:A:SER:N	9	1.23
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	6	1.23
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	6	1.23
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:VAL:N	3	1.23
(1,162)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:ALA:N	1	1.22
(1,124)	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	1:69:A:ILE:N	10	1.22
(1,29)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	9	1.22
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	6	1.22
(1,72)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:GLU:N	3	1.21
(1,69)	1:38:A:PRO:C	1:39:A:PHE:N	1:39:A:PHE:CA	1:39:A:PHE:C	5	1.21
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	4	1.21
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	1	1.19
(1,45)	1:24:A:ASP:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	2	1.19
(1,30)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:ASN:N	7	1.19
(1,172)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:ILE:N	2	1.18
(1,139)	1:78:A:TYR:C	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	1	1.17
(1,29)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	7	1.17
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	9	1.17
(1,159)	1:91:A:ASN:C	1:92:A:ASP:N	1:92:A:ASP:CA	1:92:A:ASP:C	4	1.16
(1,157)	1:90:A:ALA:C	1:91:A:ASN:N	1:91:A:ASN:CA	1:91:A:ASN:C	9	1.16
(1,147)	1:84:A:VAL:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	9	1.16
(1,24)	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	1:15:A:ILE:N	10	1.16
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	1	1.15
(1,31)	1:17:A:GLN:C	1:18:A:ASN:N	1:18:A:ASN:CA	1:18:A:ASN:C	7	1.15
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	4	1.14
(1,169)	1:96:A:LYS:C	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	2	1.13
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	2	1.13
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	4	1.13
(1,100)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:ASP:N	8	1.13
(1,92)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:PHE:N	6	1.13
(1,67)	1:37:A:ALA:C	1:38:A:PRO:N	1:38:A:PRO:CA	1:38:A:PRO:C	10	1.13
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	10	1.13
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	5	1.13
(1,29)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	3	1.13
(1,156)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ASN:N	1	1.12
(1,45)	1:24:A:ASP:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	7	1.12
(1,2)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:ILE:N	1	1.12
(1,142)	1:80:A:ASN:N	1:80:A:ASN:CA	1:80:A:ASN:C	1:81:A:GLY:N	3	1.11
(1,105)	1:57:A:VAL:C	1:58:A:ASP:N	1:58:A:ASP:CA	1:58:A:ASP:C	3	1.11
(1,91)	1:50:A:MET:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	2	1.11
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	8	1.11
(1,4)	1:4:A:ILE:N	1:4:A:ILE:CA	1:4:A:ILE:C	1:5:A:VAL:N	4	1.11
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	2	1.1
(1,162)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:ALA:N	2	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:42:A:GLU:N	1:42:A:GLU:CA	1:42:A:GLU:C	1:43:A:CYS:N	4	1.1
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	3	1.1
(1,179)	1:101:A:LYS:C	1:102:A:TYR:N	1:102:A:TYR:CA	1:102:A:TYR:C	1	1.09
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	2	1.09
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	7	1.09
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	6	1.09
(1,2)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:ILE:N	10	1.09
(1,175)	1:99:A:ILE:C	1:100:A:GLU:N	1:100:A:GLU:CA	1:100:A:GLU:C	7	1.08
(1,78)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:SER:N	8	1.08
(1,27)	1:15:A:ILE:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	2	1.08
(1,78)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:SER:N	1	1.07
(1,30)	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	1:18:A:ASN:N	1	1.07
(1,27)	1:15:A:ILE:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1	1.07
(1,1)	1:2:A:VAL:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	4	1.07
(1,91)	1:50:A:MET:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1	1.06
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	4	1.06
(1,58)	1:33:A:CYS:N	1:33:A:CYS:CA	1:33:A:CYS:C	1:34:A:LYS:N	8	1.06
(1,27)	1:15:A:ILE:C	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	6	1.06
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	3	1.05
(1,139)	1:78:A:TYR:C	1:79:A:LYS:N	1:79:A:LYS:CA	1:79:A:LYS:C	3	1.05
(1,91)	1:50:A:MET:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	4	1.05
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	5	1.05
(1,91)	1:50:A:MET:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	9	1.04
(1,54)	1:30:A:CYS:N	1:30:A:CYS:CA	1:30:A:CYS:C	1:31:A:GLY:N	10	1.04
(1,1)	1:2:A:VAL:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	7	1.04
(1,161)	1:92:A:ASP:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	9	1.03
(1,156)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:ASN:N	7	1.03
(1,36)	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1:21:A:VAL:N	8	1.03
(1,28)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:GLN:N	8	1.03
(1,18)	1:11:A:PHE:N	1:11:A:PHE:CA	1:11:A:PHE:C	1:12:A:ASP:N	4	1.03
(1,12)	1:8:A:GLN:N	1:8:A:GLN:CA	1:8:A:GLN:C	1:9:A:SER:N	5	1.03
(1,168)	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	1:97:A:GLN:N	1	1.02
(1,24)	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	1:15:A:ILE:N	2	1.02
(1,24)	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	1:15:A:ILE:N	6	1.02
(1,171)	1:97:A:GLN:C	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	6	1.01
(1,169)	1:96:A:LYS:C	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	3	1.01
(1,123)	1:67:A:GLU:C	1:68:A:ASN:N	1:68:A:ASN:CA	1:68:A:ASN:C	7	1.01
(1,83)	1:45:A:LYS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	2	1.01
(1,55)	1:31:A:GLY:C	1:32:A:PRO:N	1:32:A:PRO:CA	1:32:A:PRO:C	6	1.01
(1,29)	1:16:A:SER:C	1:17:A:GLN:N	1:17:A:GLN:CA	1:17:A:GLN:C	8	1.01
(1,10)	1:7:A:SER:N	1:7:A:SER:CA	1:7:A:SER:C	1:8:A:GLN:N	7	1.01
(1,174)	1:99:A:ILE:N	1:99:A:ILE:CA	1:99:A:ILE:C	1:100:A:GLU:N	5	1.0
(1,88)	1:48:A:THR:N	1:48:A:THR:CA	1:48:A:THR:C	1:49:A:LYS:N	10	1.0