



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 05:29 PM EST

PDB ID : 7DHT  
BMRB ID : 36397  
Title : Solution structure of ATG8f of Arabidopsis thaliana  
Authors : Lee, K.M.; Sun, S.L.; Wong, K.B.  
Deposited on : 2020-11-17

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

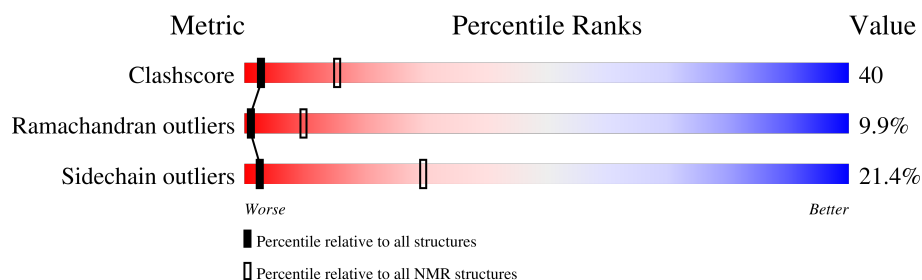
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 75%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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  $\geq 3$ , 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	121	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:12-A:115 (104)	0.52	9

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1965 atoms, of which 993 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Autophagy-related protein 8f.

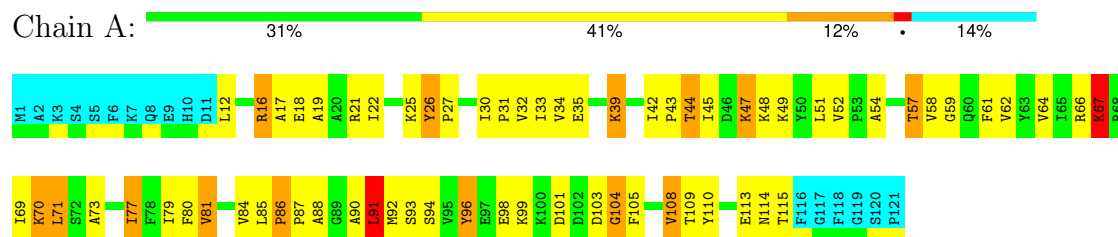
Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1965	626	993	162	182	2	

## 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: Autophagy-related protein 8f

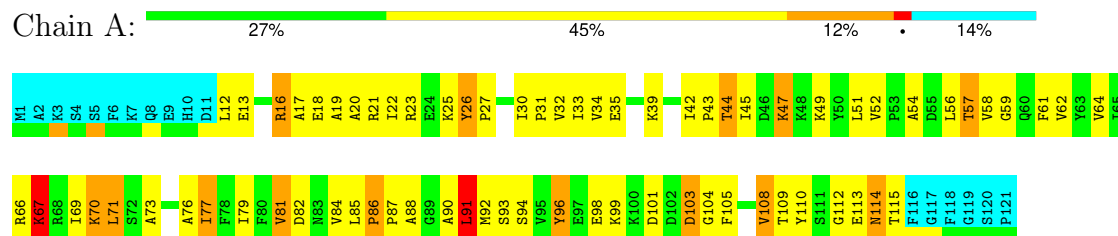


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

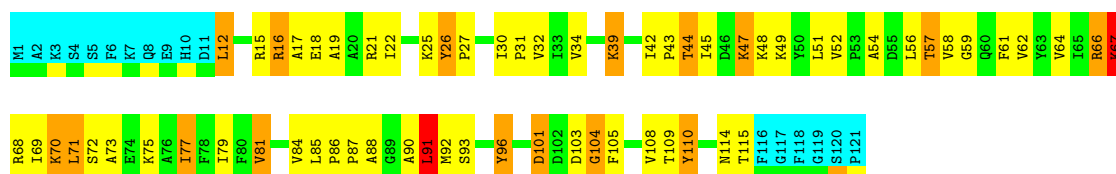
- Molecule 1: Autophagy-related protein 8f



#### 4.2.2 Score per residue for model 2

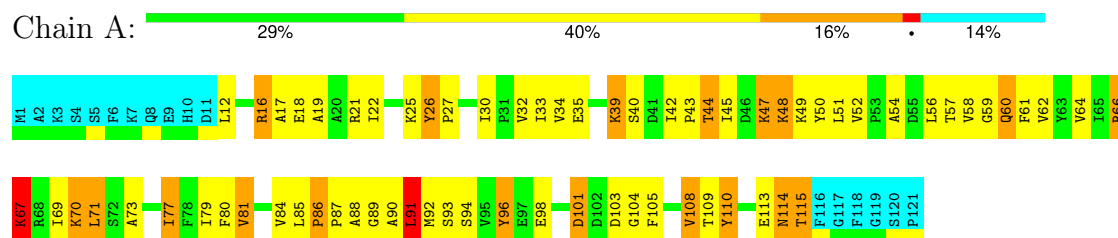
- Molecule 1: Autophagy-related protein 8f





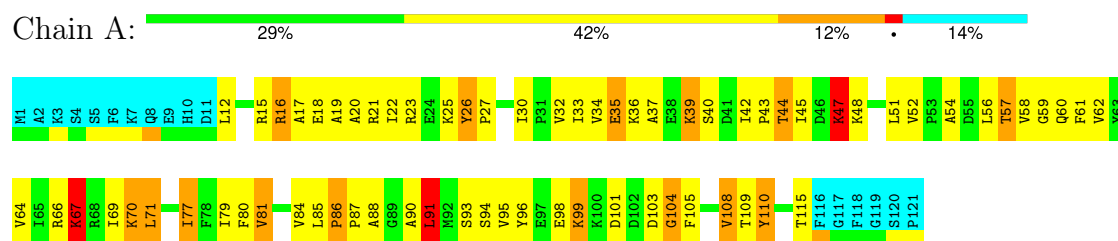
### 4.2.3 Score per residue for model 3

- Molecule 1: Autophagy-related protein 8f



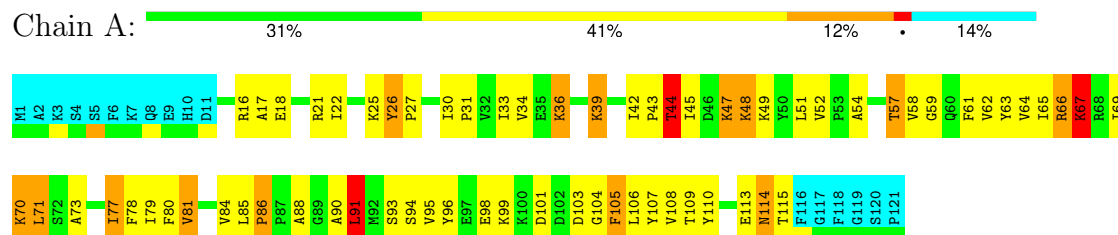
### 4.2.4 Score per residue for model 4

- Molecule 1: Autophagy-related protein 8f



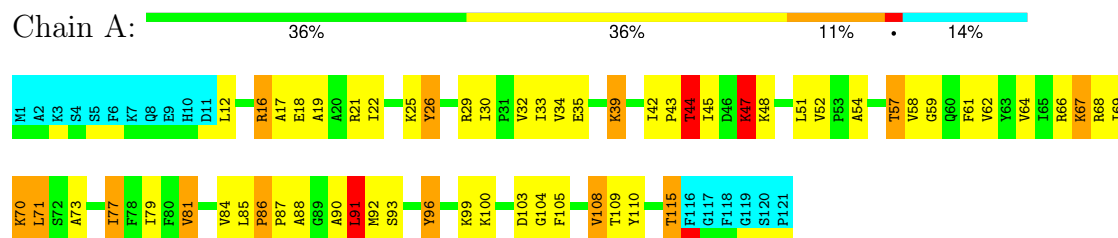
### 4.2.5 Score per residue for model 5

- Molecule 1: Autophagy-related protein 8f



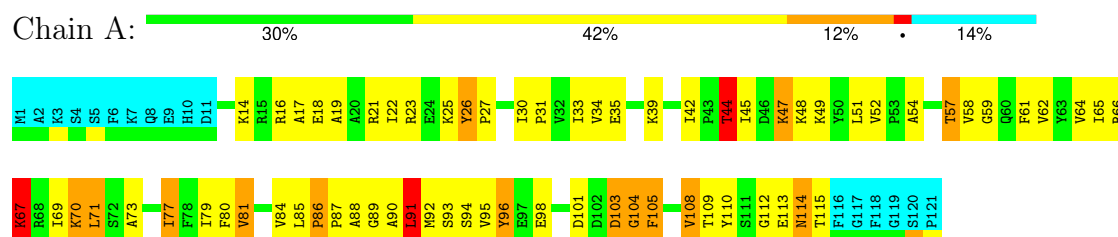
### 4.2.6 Score per residue for model 6

- Molecule 1: Autophagy-related protein 8f



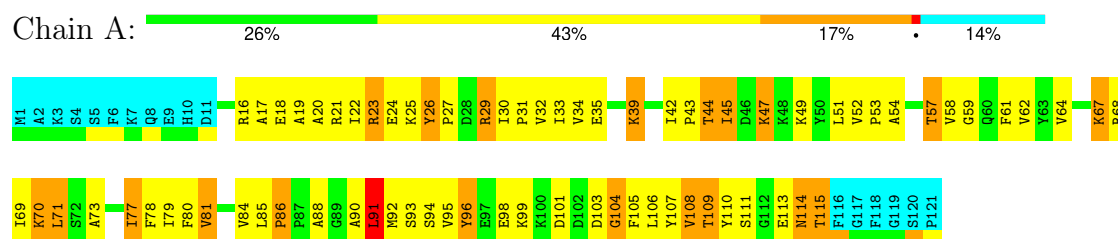
#### 4.2.7 Score per residue for model 7

- Molecule 1: Autophagy-related protein 8f



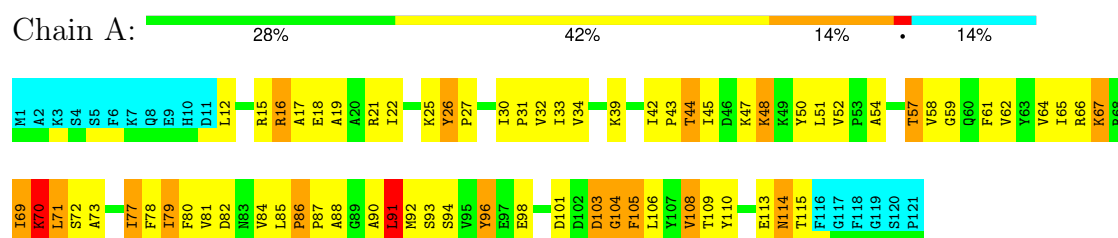
#### 4.2.8 Score per residue for model 8

- Molecule 1: Autophagy-related protein 8f



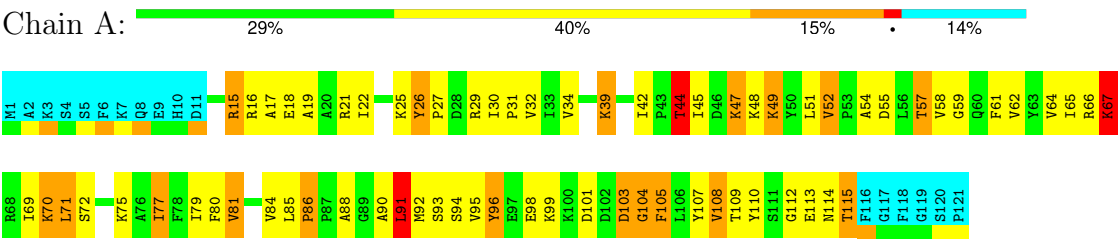
#### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Autophagy-related protein 8f



4.2.10 Score per residue for model 10

● Molecule 1: Autophagy-related protein 8f





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 9999 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	
ARIA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1264
Number of shifts mapped to atoms	1264
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

## 6 Model quality

### 6.1 Standard geometry

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

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	838	870	870	69±5
All	All	8380	8700	8700	688

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD22	1:A:115:THR:HG21	0.91	1.41	5	9
1:A:45:ILE:HB	1:A:69:ILE:HG21	0.90	1.42	3	10
1:A:69:ILE:O	1:A:71:LEU:HD23	0.85	1.71	10	9
1:A:42:ILE:CG1	1:A:71:LEU:HD21	0.79	2.06	5	9
1:A:22:ILE:HG21	1:A:51:LEU:HD21	0.77	1.56	9	9
1:A:84:VAL:HG13	1:A:86:PRO:HD3	0.73	1.60	4	9
1:A:22:ILE:HG21	1:A:51:LEU:HD11	0.72	1.61	10	1
1:A:42:ILE:HG13	1:A:71:LEU:HD21	0.72	1.61	5	8
1:A:62:VAL:HG13	1:A:77:ILE:CG1	0.71	2.15	10	10
1:A:42:ILE:HA	1:A:70:LYS:HZ1	0.69	1.48	1	7
1:A:58:VAL:HG23	1:A:90:ALA:O	0.68	1.89	3	1
1:A:57:THR:HG22	1:A:91:LEU:HD22	0.68	1.66	2	10
1:A:44:THR:HG21	1:A:70:LYS:HB3	0.67	1.66	6	1
1:A:19:ALA:HB1	1:A:104:GLY:HA3	0.66	1.66	1	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:PRO:HD2	1:A:70:LYS:HZ3	0.65	1.49	2	2
1:A:81:VAL:HG11	1:A:108:VAL:HA	0.64	1.68	8	4
1:A:39:LYS:N	1:A:39:LYS:HD3	0.64	2.07	3	9
1:A:81:VAL:HG23	1:A:84:VAL:HG12	0.63	1.69	1	9
1:A:42:ILE:O	1:A:42:ILE:HG23	0.62	1.94	7	10
1:A:71:LEU:HA	1:A:115:THR:HG21	0.62	1.69	9	2
1:A:30:ILE:N	1:A:52:VAL:O	0.62	2.33	8	10
1:A:30:ILE:HD11	1:A:93:SER:HA	0.62	1.71	3	7
1:A:62:VAL:HG13	1:A:77:ILE:HG12	0.62	1.71	10	2
1:A:42:ILE:HD12	1:A:112:GLY:HA3	0.61	1.72	10	1
1:A:45:ILE:HD12	1:A:65:ILE:HG23	0.61	1.72	5	4
1:A:42:ILE:HG12	1:A:70:LYS:HZ3	0.61	1.55	7	2
1:A:69:ILE:HG13	1:A:71:LEU:HD23	0.60	1.73	4	6
1:A:54:ALA:HB1	1:A:93:SER:HB3	0.60	1.73	7	2
1:A:30:ILE:HG22	1:A:32:VAL:HG23	0.59	1.75	3	5
1:A:42:ILE:HD11	1:A:71:LEU:HD21	0.59	1.74	6	7
1:A:30:ILE:HG22	1:A:32:VAL:HG13	0.59	1.75	8	1
1:A:22:ILE:HG21	1:A:51:LEU:CD2	0.59	2.28	3	8
1:A:67:LYS:HG3	1:A:77:ILE:HG23	0.59	1.75	8	3
1:A:56:LEU:O	1:A:91:LEU:HD13	0.59	1.98	4	1
1:A:69:ILE:HD11	1:A:110:TYR:OH	0.58	1.98	10	1
1:A:21:ARG:O	1:A:25:LYS:HB2	0.58	1.99	1	10
1:A:44:THR:HB	1:A:70:LYS:HZ1	0.57	1.58	6	1
1:A:42:ILE:CD1	1:A:71:LEU:HD21	0.57	2.30	6	8
1:A:84:VAL:HG22	1:A:85:LEU:H	0.57	1.59	7	9
1:A:35:GLU:HA	1:A:47:LYS:HD2	0.57	1.75	7	4
1:A:69:ILE:C	1:A:71:LEU:N	0.57	2.57	9	1
1:A:58:VAL:HB	1:A:88:ALA:HA	0.57	1.77	1	10
1:A:81:VAL:O	1:A:84:VAL:HG12	0.56	2.00	3	9
1:A:25:LYS:O	1:A:26:TYR:HB2	0.56	1.99	4	10
1:A:69:ILE:O	1:A:70:LYS:HG3	0.56	1.99	2	7
1:A:67:LYS:HB3	1:A:77:ILE:HG23	0.56	1.76	9	2
1:A:43:PRO:HD2	1:A:70:LYS:HZ1	0.56	1.60	8	4
1:A:95:VAL:HA	1:A:98:GLU:HB2	0.56	1.75	4	5
1:A:20:ALA:HA	1:A:23:ARG:HG2	0.55	1.77	8	3
1:A:66:ARG:HG3	1:A:68:ARG:HG2	0.55	1.78	2	1
1:A:81:VAL:HG23	1:A:84:VAL:CG1	0.55	2.31	3	9
1:A:20:ALA:HA	1:A:23:ARG:CG	0.55	2.32	4	2
1:A:12:LEU:HG	1:A:16:ARG:HB2	0.55	1.77	2	2
1:A:34:VAL:HG13	1:A:110:TYR:HB2	0.55	1.79	10	1
1:A:34:VAL:O	1:A:47:LYS:O	0.54	2.25	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD13	1:A:72:SER:N	0.54	2.17	9	1
1:A:67:LYS:O	1:A:71:LEU:HB2	0.54	2.02	8	7
1:A:44:THR:HG22	1:A:69:ILE:HB	0.54	1.79	5	3
1:A:39:LYS:HB2	1:A:39:LYS:NZ	0.54	2.17	3	2
1:A:19:ALA:HB1	1:A:104:GLY:CA	0.54	2.32	1	3
1:A:17:ALA:O	1:A:21:ARG:HB3	0.54	2.02	9	10
1:A:54:ALA:HB1	1:A:93:SER:HB2	0.54	1.80	3	8
1:A:92:MET:O	1:A:96:TYR:HB3	0.54	2.03	1	8
1:A:43:PRO:HD2	1:A:70:LYS:NZ	0.53	2.18	3	7
1:A:47:LYS:HZ2	1:A:48:LYS:HA	0.52	1.64	2	1
1:A:59:GLY:N	1:A:88:ALA:HA	0.52	2.18	4	10
1:A:36:LYS:H	1:A:36:LYS:HD3	0.52	1.63	5	1
1:A:91:LEU:HD12	1:A:93:SER:OG	0.52	2.05	9	2
1:A:57:THR:HA	1:A:91:LEU:HA	0.52	1.80	4	9
1:A:45:ILE:HG21	1:A:110:TYR:HE1	0.52	1.65	4	1
1:A:113:GLU:C	1:A:115:THR:H	0.51	2.08	10	2
1:A:80:PHE:O	1:A:109:THR:HB	0.51	2.05	5	2
1:A:71:LEU:HA	1:A:115:THR:HG23	0.51	1.82	4	1
1:A:95:VAL:HG13	1:A:99:LYS:HG2	0.51	1.82	10	4
1:A:22:ILE:HG21	1:A:51:LEU:CD1	0.51	2.35	10	1
1:A:34:VAL:HG12	1:A:110:TYR:CD1	0.51	2.40	7	2
1:A:62:VAL:HG13	1:A:77:ILE:HG13	0.51	1.82	8	10
1:A:65:ILE:HD13	1:A:110:TYR:CE1	0.51	2.39	10	1
1:A:69:ILE:O	1:A:71:LEU:N	0.51	2.44	9	1
1:A:91:LEU:HD12	1:A:93:SER:HB3	0.51	1.83	3	5
1:A:33:ILE:O	1:A:108:VAL:O	0.50	2.30	7	7
1:A:79:ILE:O	1:A:85:LEU:HD23	0.50	2.07	9	1
1:A:113:GLU:O	1:A:115:THR:N	0.50	2.44	1	4
1:A:35:GLU:OE1	1:A:47:LYS:HE3	0.50	2.07	1	1
1:A:58:VAL:HG11	1:A:86:PRO:CB	0.50	2.36	4	8
1:A:12:LEU:O	1:A:16:ARG:HB2	0.50	2.07	6	4
1:A:67:LYS:HB2	1:A:71:LEU:HG	0.50	1.84	9	1
1:A:69:ILE:C	1:A:71:LEU:H	0.50	2.09	9	1
1:A:69:ILE:O	1:A:69:ILE:HG13	0.50	2.07	9	2
1:A:61:PHE:O	1:A:64:VAL:HB	0.50	2.07	1	10
1:A:47:LYS:HE2	1:A:48:LYS:H	0.50	1.67	4	4
1:A:35:GLU:O	1:A:109:THR:HG23	0.50	2.06	7	3
1:A:84:VAL:HG12	1:A:85:LEU:N	0.50	2.22	2	1
1:A:71:LEU:HA	1:A:115:THR:CG2	0.49	2.36	9	1
1:A:70:LYS:O	1:A:70:LYS:HD2	0.49	2.07	9	1
1:A:80:PHE:CE1	1:A:85:LEU:HG	0.49	2.42	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:HG23	1:A:110:TYR:CE2	0.49	2.42	6	2
1:A:54:ALA:HB1	1:A:93:SER:CB	0.49	2.38	3	8
1:A:42:ILE:HD11	1:A:71:LEU:HD23	0.49	1.84	9	1
1:A:19:ALA:O	1:A:22:ILE:HG12	0.48	2.08	1	3
1:A:113:GLU:O	1:A:114:ASN:C	0.48	2.52	8	4
1:A:16:ARG:HD3	1:A:103:ASP:HB2	0.48	1.86	1	1
1:A:25:LYS:O	1:A:26:TYR:CB	0.48	2.62	6	10
1:A:18:GLU:HA	1:A:21:ARG:HG2	0.47	1.86	4	8
1:A:91:LEU:O	1:A:95:VAL:HB	0.47	2.09	7	5
1:A:34:VAL:O	1:A:47:LYS:HB2	0.47	2.09	4	6
1:A:47:LYS:HZ2	1:A:48:LYS:CA	0.47	2.22	2	1
1:A:113:GLU:C	1:A:115:THR:N	0.47	2.67	10	3
1:A:35:GLU:O	1:A:110:TYR:N	0.47	2.47	7	3
1:A:58:VAL:HG21	1:A:87:PRO:HD2	0.47	1.86	4	2
1:A:69:ILE:HG13	1:A:71:LEU:CD2	0.47	2.40	6	1
1:A:30:ILE:HD12	1:A:106:LEU:HD22	0.47	1.86	8	1
1:A:84:VAL:HG22	1:A:85:LEU:N	0.47	2.24	9	9
1:A:32:VAL:O	1:A:33:ILE:HD13	0.47	2.10	8	1
1:A:12:LEU:O	1:A:13:GLU:C	0.47	2.53	1	1
1:A:45:ILE:HB	1:A:69:ILE:CG2	0.47	2.37	9	3
1:A:67:LYS:CG	1:A:77:ILE:HG23	0.46	2.40	2	2
1:A:114:ASN:HD22	1:A:114:ASN:N	0.46	2.07	3	1
1:A:31:PRO:HB3	1:A:105:PHE:CE2	0.46	2.46	10	3
1:A:77:ILE:HD13	1:A:110:TYR:CE1	0.46	2.45	10	1
1:A:18:GLU:O	1:A:22:ILE:HG23	0.46	2.11	7	5
1:A:12:LEU:HA	1:A:15:ARG:HB3	0.46	1.85	2	2
1:A:45:ILE:HG21	1:A:110:TYR:CE1	0.46	2.45	4	1
1:A:33:ILE:HG23	1:A:49:LYS:HG3	0.46	1.85	5	1
1:A:12:LEU:HG	1:A:12:LEU:O	0.46	2.11	2	1
1:A:25:LYS:HB3	1:A:27:PRO:HD2	0.46	1.87	4	8
1:A:70:LYS:HD2	1:A:70:LYS:C	0.46	2.31	2	4
1:A:87:PRO:O	1:A:88:ALA:C	0.46	2.54	3	6
1:A:35:GLU:HB2	1:A:109:THR:OG1	0.46	2.11	8	1
1:A:67:LYS:NZ	1:A:76:ALA:HB1	0.45	2.26	1	1
1:A:42:ILE:HG23	1:A:110:TYR:HE2	0.45	1.69	6	1
1:A:94:SER:O	1:A:98:GLU:N	0.45	2.49	3	8
1:A:34:VAL:HG12	1:A:47:LYS:HB3	0.45	1.88	6	1
1:A:47:LYS:HD3	1:A:48:LYS:H	0.45	1.72	6	1
1:A:44:THR:CG2	1:A:70:LYS:HB3	0.45	2.39	6	1
1:A:19:ALA:O	1:A:23:ARG:HG2	0.45	2.12	1	2
1:A:37:ALA:HB3	1:A:40:SER:HB3	0.45	1.89	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ARG:O	1:A:67:LYS:C	0.45	2.55	9	7
1:A:96:TYR:O	1:A:101:ASP:HB3	0.45	2.12	2	3
1:A:60:GLN:HE21	1:A:60:GLN:HA	0.45	1.72	3	1
1:A:58:VAL:HG11	1:A:86:PRO:HB2	0.45	1.87	4	4
1:A:61:PHE:HB2	1:A:92:MET:SD	0.45	2.52	2	6
1:A:65:ILE:HD13	1:A:110:TYR:CD1	0.45	2.47	10	1
1:A:18:GLU:O	1:A:21:ARG:HG2	0.45	2.12	5	5
1:A:29:ARG:HB3	1:A:53:PRO:HA	0.44	1.89	8	1
1:A:80:PHE:HA	1:A:84:VAL:O	0.44	2.13	9	6
1:A:47:LYS:HZ2	1:A:48:LYS:N	0.44	2.10	2	1
1:A:15:ARG:HG3	1:A:105:PHE:HB2	0.44	1.88	9	1
1:A:71:LEU:HD13	1:A:72:SER:H	0.44	1.73	9	1
1:A:16:ARG:HD3	1:A:103:ASP:HB3	0.44	1.89	9	1
1:A:45:ILE:HG21	1:A:110:TYR:CE2	0.44	2.48	2	1
1:A:47:LYS:HG3	1:A:48:LYS:H	0.44	1.73	7	1
1:A:65:ILE:HG21	1:A:110:TYR:CE1	0.44	2.48	10	1
1:A:30:ILE:HG12	1:A:54:ALA:CB	0.44	2.43	7	1
1:A:29:ARG:HD3	1:A:51:LEU:HB3	0.43	1.89	6	1
1:A:47:LYS:CD	1:A:48:LYS:H	0.43	2.26	6	1
1:A:34:VAL:HG12	1:A:110:TYR:HD2	0.43	1.73	9	1
1:A:42:ILE:HD13	1:A:110:TYR:CE2	0.43	2.49	10	1
1:A:31:PRO:O	1:A:106:LEU:O	0.43	2.36	5	1
1:A:63:TYR:O	1:A:66:ARG:HB3	0.43	2.14	5	1
1:A:58:VAL:HB	1:A:88:ALA:CA	0.43	2.42	9	6
1:A:42:ILE:HG23	1:A:110:TYR:CE1	0.43	2.48	8	3
1:A:42:ILE:HA	1:A:70:LYS:NZ	0.43	2.25	5	1
1:A:66:ARG:HG3	1:A:68:ARG:HB2	0.43	1.91	6	1
1:A:69:ILE:O	1:A:70:LYS:HB3	0.43	2.14	6	1
1:A:58:VAL:HA	1:A:92:MET:HG2	0.43	1.90	7	1
1:A:94:SER:O	1:A:98:GLU:HG3	0.42	2.14	5	1
1:A:42:ILE:HB	1:A:112:GLY:HA3	0.42	1.90	7	2
1:A:54:ALA:O	1:A:93:SER:HB2	0.42	2.14	1	2
1:A:31:PRO:HG2	1:A:105:PHE:HA	0.42	1.90	5	1
1:A:93:SER:O	1:A:94:SER:C	0.42	2.58	1	4
1:A:31:PRO:O	1:A:106:LEU:N	0.42	2.52	8	1
1:A:22:ILE:CD1	1:A:31:PRO:HG3	0.42	2.45	5	3
1:A:42:ILE:O	1:A:42:ILE:CG2	0.42	2.68	4	1
1:A:18:GLU:HB3	1:A:105:PHE:CE2	0.42	2.50	5	1
1:A:47:LYS:O	1:A:48:LYS:C	0.42	2.58	9	1
1:A:23:ARG:HG3	1:A:24:GLU:N	0.41	2.30	8	1
1:A:42:ILE:HD11	1:A:69:ILE:HD11	0.41	1.92	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:THR:HB	1:A:70:LYS:HG2	0.41	1.91	9	1
1:A:72:SER:HB2	1:A:75:LYS:HE3	0.41	1.91	10	1
1:A:26:TYR:N	1:A:27:PRO:CD	0.41	2.83	10	6
1:A:96:TYR:HA	1:A:100:LYS:O	0.41	2.15	6	1
1:A:18:GLU:HA	1:A:21:ARG:HE	0.41	1.74	7	1
1:A:77:ILE:HD12	1:A:78:PHE:N	0.41	2.30	5	2
1:A:30:ILE:O	1:A:52:VAL:HG22	0.41	2.15	8	2
1:A:43:PRO:O	1:A:44:THR:HB	0.41	2.15	5	2
1:A:26:TYR:N	1:A:27:PRO:HD2	0.41	2.30	10	2
1:A:34:VAL:O	1:A:47:LYS:NZ	0.41	2.45	2	1
1:A:56:LEU:HD13	1:A:60:GLN:HB3	0.41	1.92	4	1
1:A:30:ILE:HG22	1:A:32:VAL:CG1	0.41	2.45	10	1
1:A:72:SER:HB2	1:A:75:LYS:HB2	0.41	1.93	2	1
1:A:30:ILE:HG12	1:A:54:ALA:HB2	0.41	1.92	7	2
1:A:34:VAL:HG12	1:A:110:TYR:CD2	0.41	2.50	9	1
1:A:70:LYS:HZ2	1:A:115:THR:HG22	0.41	1.76	3	1
1:A:91:LEU:O	1:A:93:SER:N	0.40	2.54	3	1
1:A:70:LYS:HD3	1:A:115:THR:HG22	0.40	1.93	6	1
1:A:93:SER:OG	1:A:94:SER:N	0.40	2.54	9	1
1:A:45:ILE:HB	1:A:69:ILE:HD13	0.40	1.93	10	1
1:A:31:PRO:O	1:A:106:LEU:HB3	0.40	2.17	9	1
1:A:114:ASN:O	1:A:115:THR:C	0.40	2.58	9	1
1:A:93:SER:O	1:A:96:TYR:N	0.40	2.54	10	1
1:A:66:ARG:O	1:A:68:ARG:N	0.40	2.55	2	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	104/121 (86%)	75±3 (72±3%)	19±3 (18±2%)	10±1 (10±1%)	<b>1</b>	<b>10</b>
All	All	1040/1210 (86%)	747 (72%)	190 (18%)	103 (10%)	<b>1</b>	<b>10</b>

All 17 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	26	TYR	10
1	A	86	PRO	10
1	A	91	LEU	10
1	A	103	ASP	10
1	A	44	THR	9
1	A	90	ALA	9
1	A	73	ALA	8
1	A	67	LYS	7
1	A	114	ASN	7
1	A	104	GLY	7
1	A	115	THR	4
1	A	66	ARG	3
1	A	48	LYS	3
1	A	89	GLY	2
1	A	47	LYS	2
1	A	69	ILE	1
1	A	70	LYS	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/105 (87%)	72±3 (79±3%)	20±3 (21±3%)	2	29
All	All	910/1050 (87%)	715 (79%)	195 (21%)	2	29

All 41 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	16	ARG	10
1	A	44	THR	10
1	A	67	LYS	10
1	A	70	LYS	10
1	A	71	LEU	10
1	A	77	ILE	10
1	A	79	ILE	10
1	A	91	LEU	10
1	A	96	TYR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	105	PHE	10
1	A	108	VAL	10
1	A	47	LYS	9
1	A	57	THR	9
1	A	81	VAL	9
1	A	101	ASP	8
1	A	39	LYS	8
1	A	49	LYS	6
1	A	56	LEU	3
1	A	99	LYS	3
1	A	110	TYR	3
1	A	50	TYR	2
1	A	109	THR	2
1	A	36	LYS	2
1	A	23	ARG	2
1	A	103	ASP	2
1	A	29	ARG	2
1	A	12	LEU	1
1	A	40	SER	1
1	A	60	GLN	1
1	A	114	ASN	1
1	A	32	VAL	1
1	A	35	GLU	1
1	A	14	LYS	1
1	A	45	ILE	1
1	A	68	ARG	1
1	A	107	TYR	1
1	A	111	SER	1
1	A	78	PHE	1
1	A	15	ARG	1
1	A	52	VAL	1
1	A	55	ASP	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 74% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `starch_output`

#### 7.1.1 Bookkeeping [i](#)

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

Total number of shifts	1264
Number of shifts mapped to atoms	1264
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	118	$-0.00 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	111	$0.04 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	107	$-0.45 \pm 0.37$	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 75%, i.e. 1118 atoms were assigned a chemical shift out of a possible 1484. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	395/512 (77%)	198/206 (96%)	103/208 (50%)	94/98 (96%)
Sidechain	684/878 (78%)	471/569 (83%)	213/273 (78%)	0/36 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	39/94 (41%)	19/44 (43%)	20/50 (40%)	0/0 (—%)
Overall	1118/1484 (75%)	688/819 (84%)	336/531 (63%)	94/134 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1264 atoms were assigned a chemical shift out of a possible 1698. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	454/597 (76%)	229/241 (95%)	118/242 (49%)	107/114 (94%)
Sidechain	747/969 (77%)	515/627 (82%)	232/303 (77%)	0/39 (0%)
Aromatic	63/132 (48%)	31/63 (49%)	32/67 (48%)	0/2 (0%)
Overall	1264/1698 (74%)	775/931 (83%)	382/612 (62%)	107/155 (69%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

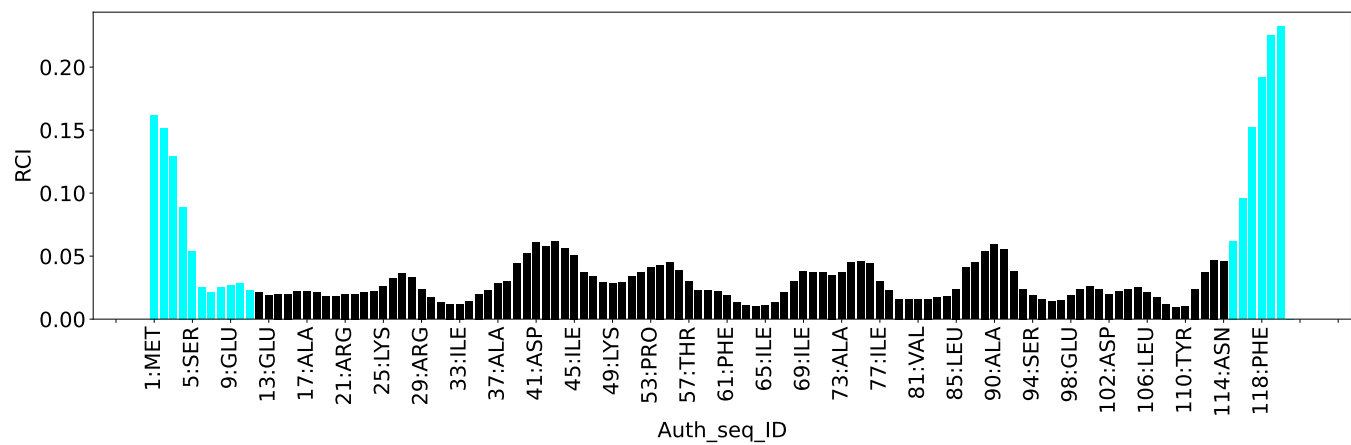
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	66	ARG	CD	36.00	38.57 – 47.75	-7.8
1	A	33	ILE	HD11	-0.95	-0.72 – 2.09	-5.8
1	A	33	ILE	HD12	-0.95	-0.72 – 2.09	-5.8
1	A	33	ILE	HD13	-0.95	-0.72 – 2.09	-5.8

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

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	1370
Intra-residue ( $ i-j =0$ )	621
Sequential ( $ i-j =1$ )	248
Medium range ( $ i-j >1$ and $ i-j <5$ )	159
Long range ( $ i-j \geq 5$ )	284
Inter-chain	0
Hydrogen bond restraints	58
Disulfide bond restraints	0
Total dihedral-angle restraints	173
Number of unmapped restraints	0
Number of restraints per residue	12.8
Number of long range restraints per residue <sup>1</sup>	2.4

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

### 8.2 Residual restraint violations

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	96.2	0.2
0.2-0.5 (Medium)	187.6	0.5
>0.5 (Large)	95.9	3.39

### 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)	17.9	4.91
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

### 9.1 Summary of distance violations ⓘ

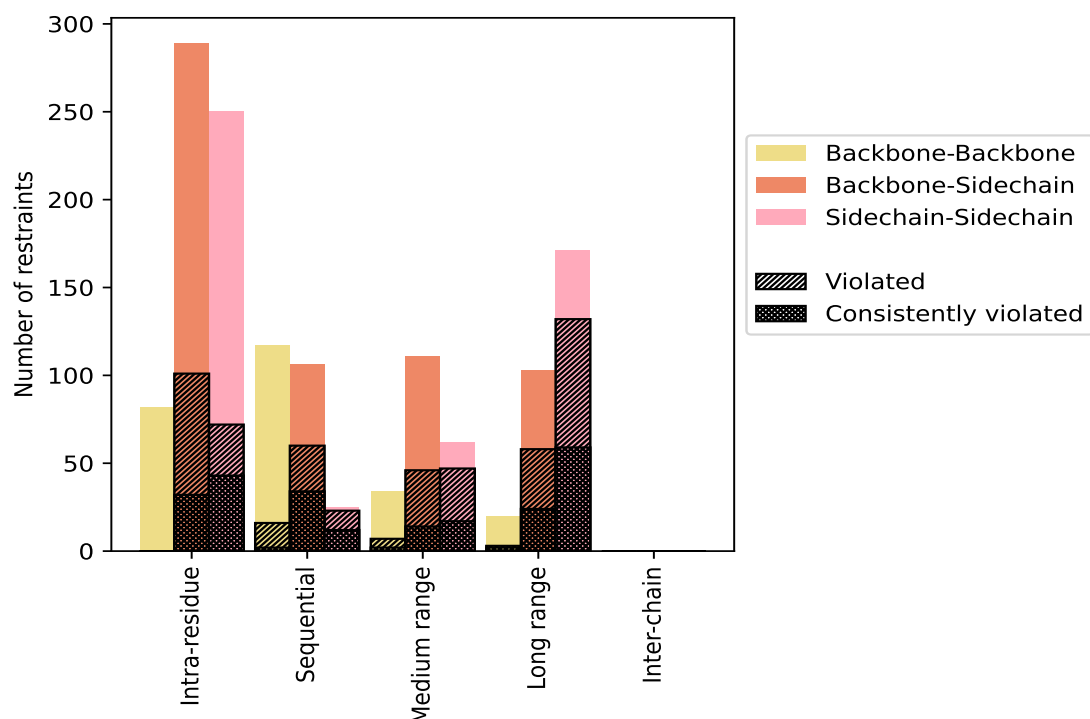
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>621</b>	<b>45.3</b>	<b>173</b>	<b>27.9</b>	<b>12.6</b>	<b>75</b>	<b>12.1</b>	<b>5.5</b>
Backbone-Backbone	82	6.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	289	21.1	101	34.9	7.4	32	11.1	2.3
Sidechain-Sidechain	250	18.2	72	28.8	5.3	43	17.2	3.1
<b>Sequential (<math> i-j =1</math>)</b>	<b>248</b>	<b>18.1</b>	<b>99</b>	<b>39.9</b>	<b>7.2</b>	<b>48</b>	<b>19.4</b>	<b>3.5</b>
Backbone-Backbone	117	8.5	16	13.7	1.2	2	1.7	0.1
Backbone-Sidechain	106	7.7	60	56.6	4.4	34	32.1	2.5
Sidechain-Sidechain	25	1.8	23	92.0	1.7	12	48.0	0.9
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>159</b>	<b>11.6</b>	<b>87</b>	<b>54.7</b>	<b>6.4</b>	<b>32</b>	<b>20.1</b>	<b>2.3</b>
Backbone-Backbone	34	2.5	7	20.6	0.5	2	5.9	0.1
Backbone-Sidechain	63	4.6	33	52.4	2.4	13	20.6	0.9
Sidechain-Sidechain	62	4.5	47	75.8	3.4	17	27.4	1.2
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>284</b>	<b>20.7</b>	<b>189</b>	<b>66.5</b>	<b>13.8</b>	<b>85</b>	<b>29.9</b>	<b>6.2</b>
Backbone-Backbone	20	1.5	3	15.0	0.2	2	10.0	0.1
Backbone-Sidechain	93	6.8	54	58.1	3.9	24	25.8	1.8
Sidechain-Sidechain	171	12.5	132	77.2	9.6	59	34.5	4.3
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>58</b>	<b>4.2</b>	<b>17</b>	<b>29.3</b>	<b>1.2</b>	<b>1</b>	<b>1.7</b>	<b>0.1</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1370</b>	<b>100.0</b>	<b>565</b>	<b>41.2</b>	<b>41.2</b>	<b>241</b>	<b>17.6</b>	<b>17.6</b>
Backbone-Backbone	253	18.5	26	10.3	1.9	6	2.4	0.4
Backbone-Sidechain	609	44.5	265	43.5	19.3	104	17.1	7.6
Sidechain-Sidechain	508	37.1	274	53.9	20.0	131	25.8	9.6

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

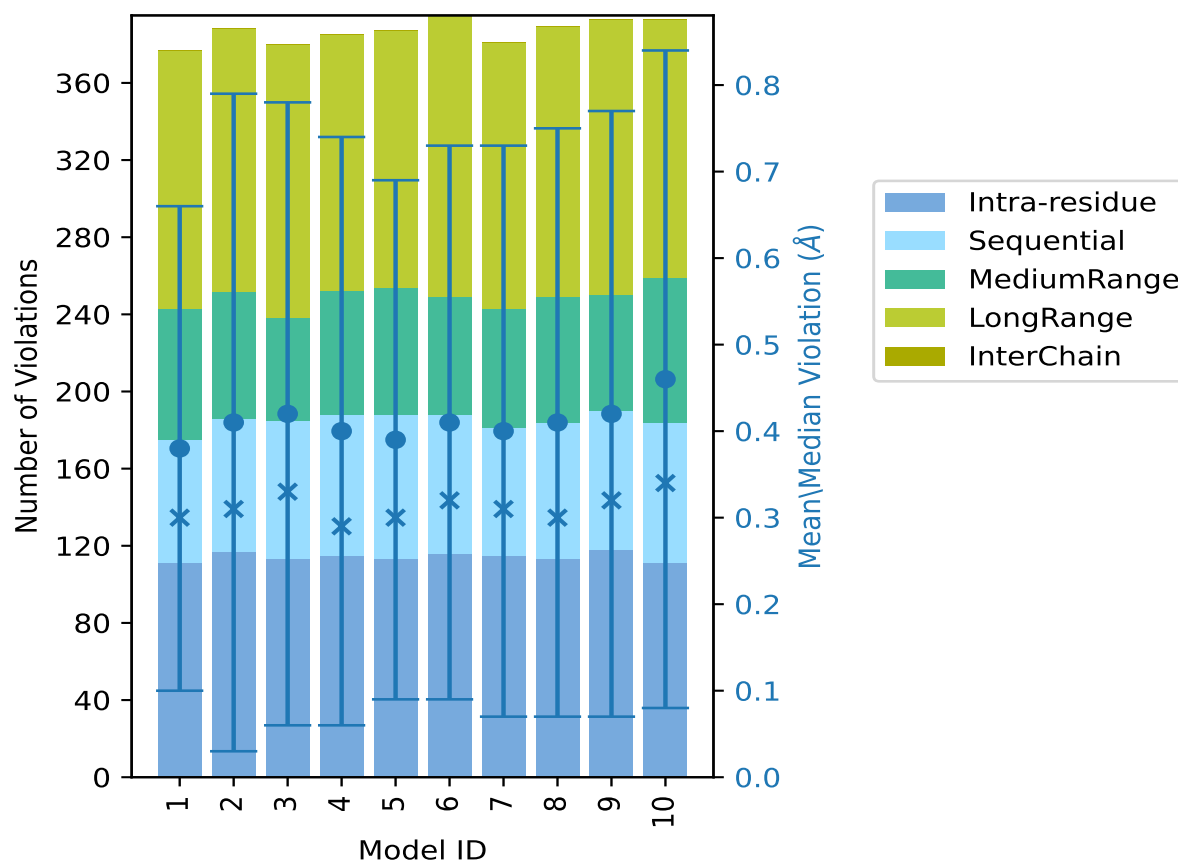
## 9.2 Distance violation statistics for each model [i](#)

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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	111	64	68	134	0	377	0.38	1.83	0.28	0.3
2	117	69	66	136	0	388	0.41	3.16	0.38	0.31
3	113	72	53	142	0	380	0.42	3.28	0.36	0.33
4	115	73	64	133	0	385	0.4	3.39	0.34	0.29
5	113	75	66	133	0	387	0.39	2.0	0.3	0.3
6	116	72	61	146	0	395	0.41	2.04	0.32	0.32
7	115	66	62	138	0	381	0.4	2.74	0.33	0.31
8	113	71	65	140	0	389	0.41	2.48	0.34	0.3
9	118	72	60	143	0	393	0.42	3.23	0.35	0.32
10	111	73	75	134	0	393	0.46	2.25	0.38	0.34

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard 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, 764(IR:448, SQ:149, MR:72, LR:95, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
30	12	12	23	0	77	1	10.0
10	3	7	16	0	36	2	20.0
9	8	4	4	0	25	3	30.0

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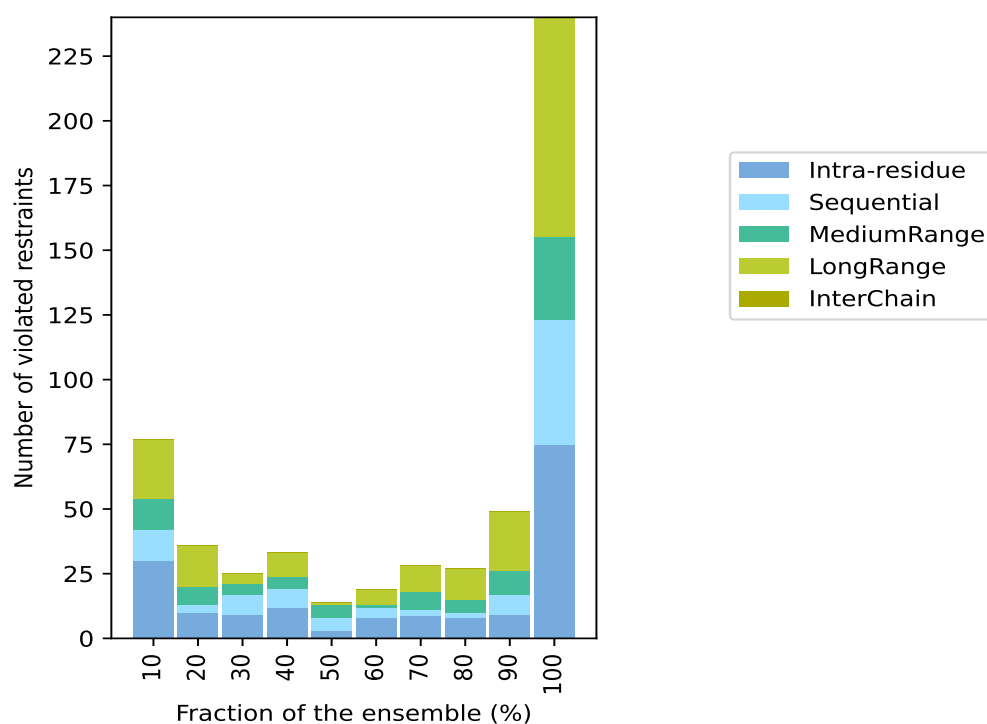
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
12	7	5	9	0	33	4	40.0
3	5	5	1	0	14	5	50.0
8	4	1	6	0	19	6	60.0
9	2	7	10	0	28	7	70.0
8	2	5	12	0	27	8	80.0
9	8	9	23	0	49	9	90.0
75	48	32	85	0	240	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

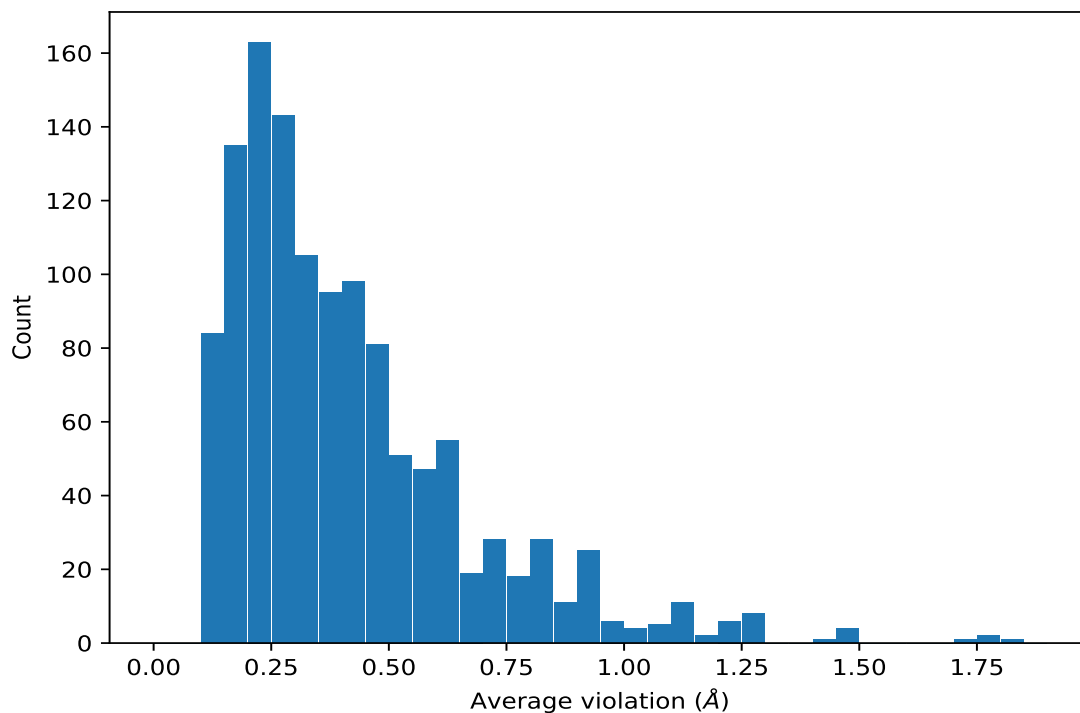


## 9.4 Most violated distance restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	10	1.82	0.09	1.82
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	10	1.73	0.04	1.74
(2,775)	1:58:A:VAL:HG13	1:61:A:PHE:HB2	10	1.48	0.09	1.48
(2,775)	1:58:A:VAL:HG12	1:61:A:PHE:HB2	10	1.48	0.09	1.48
(2,775)	1:58:A:VAL:HG11	1:61:A:PHE:HB2	10	1.48	0.09	1.48
(2,852)	1:20:A:ALA:HB1	1:23:A:ARG:HG3	10	1.28	0.45	1.55
(2,852)	1:20:A:ALA:HB3	1:23:A:ARG:HG3	10	1.28	0.45	1.55
(2,852)	1:20:A:ALA:HB2	1:23:A:ARG:HG3	10	1.28	0.45	1.55
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	10	1.28	0.03	1.27
(2,774)	1:57:A:THR:HG23	1:89:A:GLY:HA3	10	1.28	0.03	1.27
(2,774)	1:57:A:THR:HG21	1:89:A:GLY:HA3	10	1.28	0.03	1.27
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	10	1.16	0.53	0.99
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB2	10	1.16	0.53	0.99
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG23	10	1.14	0.1	1.12
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	10	1.14	0.1	1.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,818)	1:54:A:ALA:HB1	1:28:A:ASP:HB3	10	1.1	0.82	0.51
(2,818)	1:54:A:ALA:HB2	1:28:A:ASP:HB3	10	1.1	0.82	0.51
(2,818)	1:54:A:ALA:HB3	1:28:A:ASP:HB3	10	1.1	0.82	0.51
(1,233)	1:84:A:VAL:HG22	1:86:A:PRO:HD2	10	1.09	0.83	0.9
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	10	1.09	0.83	0.9
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	10	1.07	0.68	0.74
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA2	10	1.07	0.68	0.74
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	10	1.06	0.05	1.06
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG23	10	0.95	0.14	0.98
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG21	10	0.95	0.14	0.98
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG22	10	0.95	0.14	0.98
(1,95)	1:90:A:ALA:HA	1:95:A:VAL:HG21	10	0.95	0.14	0.98
(1,95)	1:90:A:ALA:HA	1:95:A:VAL:HG22	10	0.95	0.14	0.98
(1,228)	1:32:A:VAL:HG23	1:106:A:LEU:HD21	10	0.91	0.34	0.84
(1,228)	1:32:A:VAL:HG21	1:106:A:LEU:HD22	10	0.91	0.34	0.84
(1,228)	1:32:A:VAL:HG22	1:106:A:LEU:HD23	10	0.91	0.34	0.84
(1,228)	1:32:A:VAL:HG23	1:106:A:LEU:HD22	10	0.91	0.34	0.84
(1,228)	1:32:A:VAL:HG21	1:106:A:LEU:HD23	10	0.91	0.34	0.84
(1,228)	1:32:A:VAL:HG21	1:106:A:LEU:HD21	10	0.91	0.34	0.84
(1,228)	1:30:A:ILE:HG13	1:52:A:VAL:HG22	10	0.91	0.34	0.84
(1,228)	1:30:A:ILE:HG13	1:52:A:VAL:HG23	10	0.91	0.34	0.84
(1,228)	1:30:A:ILE:HG13	1:52:A:VAL:HG21	10	0.91	0.34	0.84
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG22	10	0.91	0.03	0.92
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG21	10	0.91	0.03	0.92
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG23	10	0.91	0.03	0.92
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG11	10	0.9	1.01	0.27
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG12	10	0.9	1.01	0.27
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG13	10	0.9	1.01	0.27
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	10	0.86	0.07	0.86
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD12	10	0.85	0.08	0.83
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	10	0.85	0.08	0.83
(2,860)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	10	0.85	0.08	0.83
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	10	0.84	0.34	0.96
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	10	0.83	0.08	0.86
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG22	10	0.83	0.08	0.86
(2,822)	1:76:A:ALA:HB1	1:67:A:LYS:HD3	10	0.82	0.33	0.87
(2,822)	1:76:A:ALA:HB2	1:67:A:LYS:HD3	10	0.82	0.33	0.87
(2,822)	1:76:A:ALA:HB3	1:67:A:LYS:HD3	10	0.82	0.33	0.87
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD12	10	0.8	0.14	0.74
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD11	10	0.8	0.14	0.74
(1,168)	1:62:A:VAL:HG12	1:65:A:ILE:HD12	10	0.8	0.14	0.74
(1,168)	1:62:A:VAL:HG12	1:65:A:ILE:HD11	10	0.8	0.14	0.74

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,168)	1:62:A:VAL:HG11	1:65:A:ILE:HD11	10	0.8	0.14	0.74
(2,898)	1:65:A:ILE:HD12	1:61:A:PHE:HD2	10	0.8	0.19	0.86
(2,898)	1:65:A:ILE:HD11	1:61:A:PHE:HD2	10	0.8	0.19	0.86
(2,898)	1:65:A:ILE:HD12	1:61:A:PHE:HD1	10	0.8	0.19	0.86
(2,898)	1:65:A:ILE:HD11	1:61:A:PHE:HD1	10	0.8	0.19	0.86
(2,898)	1:65:A:ILE:HD13	1:61:A:PHE:HD2	10	0.8	0.19	0.86
(1,162)	1:32:A:VAL:HG23	1:106:A:LEU:HB3	10	0.8	0.79	0.34
(1,162)	1:32:A:VAL:HG21	1:106:A:LEU:HB3	10	0.8	0.79	0.34
(1,162)	1:32:A:VAL:HG22	1:106:A:LEU:HB3	10	0.8	0.79	0.34
(1,162)	1:52:A:VAL:HG22	1:92:A:MET:HB2	10	0.8	0.79	0.34
(1,162)	1:52:A:VAL:HG23	1:29:A:ARG:HB2	10	0.8	0.79	0.34
(1,162)	1:52:A:VAL:HG21	1:92:A:MET:HB2	10	0.8	0.79	0.34
(2,742)	1:34:A:VAL:HG11	1:34:A:VAL:H	10	0.79	0.02	0.78
(2,742)	1:34:A:VAL:HG13	1:34:A:VAL:H	10	0.79	0.02	0.78
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	10	0.78	0.04	0.78
(1,125)	1:65:A:ILE:HB	1:45:A:ILE:HD11	10	0.78	0.04	0.78
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG11	10	0.77	0.13	0.76
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG12	10	0.77	0.13	0.76
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG13	10	0.77	0.13	0.76
(1,191)	1:65:A:ILE:HG21	1:45:A:ILE:HG23	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG21	1:45:A:ILE:HG22	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG23	1:45:A:ILE:HG21	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG22	1:42:A:ILE:HD12	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG23	1:42:A:ILE:HD12	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG22	1:42:A:ILE:HD13	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG22	1:45:A:ILE:HG23	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG21	1:42:A:ILE:HD13	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG21	1:42:A:ILE:HD11	10	0.77	0.31	0.68
(1,191)	1:65:A:ILE:HG23	1:45:A:ILE:HG23	10	0.77	0.31	0.68
(1,234)	1:88:A:ALA:HB2	1:58:A:VAL:HB	10	0.74	0.03	0.75
(1,234)	1:88:A:ALA:HB3	1:58:A:VAL:HB	10	0.74	0.03	0.75
(1,234)	1:88:A:ALA:HB1	1:58:A:VAL:HB	10	0.74	0.03	0.75
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	10	0.74	0.03	0.74
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD13	10	0.73	0.13	0.77
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD11	10	0.73	0.13	0.77
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD12	10	0.73	0.13	0.77
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD11	10	0.72	0.31	0.71
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD12	10	0.72	0.31	0.71
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD13	10	0.72	0.31	0.71
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG23	10	0.72	0.04	0.72
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG22	10	0.72	0.04	0.72
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG21	10	0.72	0.04	0.72

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD21	10	0.71	0.22	0.69
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD23	10	0.71	0.22	0.69
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD22	10	0.71	0.22	0.69
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB1	10	0.71	0.1	0.72
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB3	10	0.71	0.1	0.72
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB2	10	0.71	0.1	0.72
(2,739)	1:108:A:VAL:HG13	1:108:A:VAL:H	10	0.71	0.04	0.7
(2,739)	1:108:A:VAL:HG11	1:108:A:VAL:H	10	0.71	0.04	0.7
(2,739)	1:108:A:VAL:HG12	1:108:A:VAL:H	10	0.71	0.04	0.7
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	10	0.7	0.03	0.7
(2,776)	1:12:A:LEU:HD11	1:16:A:ARG:HD3	10	0.7	0.39	0.46
(2,776)	1:12:A:LEU:HD13	1:16:A:ARG:HD2	10	0.7	0.39	0.46
(2,776)	1:12:A:LEU:HD12	1:16:A:ARG:HD3	10	0.7	0.39	0.46
(2,776)	1:12:A:LEU:HD13	1:16:A:ARG:HD3	10	0.7	0.39	0.46
(1,155)	1:44:A:THR:H	1:44:A:THR:HG21	10	0.68	0.09	0.72
(1,155)	1:44:A:THR:H	1:44:A:THR:HG23	10	0.68	0.09	0.72
(1,155)	1:44:A:THR:H	1:44:A:THR:HG22	10	0.68	0.09	0.72
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB3	10	0.67	0.08	0.68
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB1	10	0.67	0.08	0.68
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	10	0.66	0.39	0.64
(2,842)	1:30:A:ILE:HG21	1:96:A:TYR:HB2	10	0.66	0.1	0.62
(2,842)	1:30:A:ILE:HG22	1:96:A:TYR:HB2	10	0.66	0.1	0.62
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG11	10	0.65	0.02	0.65
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG13	10	0.65	0.02	0.65
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG12	10	0.65	0.02	0.65
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD13	10	0.64	0.05	0.64
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD12	10	0.64	0.05	0.64
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD11	10	0.64	0.05	0.64
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD11	10	0.64	0.37	0.48
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD13	10	0.64	0.37	0.48
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD12	10	0.64	0.37	0.48
(1,137)	1:45:A:ILE:HG12	1:69:A:ILE:HD11	10	0.64	0.09	0.62
(1,137)	1:45:A:ILE:HG13	1:69:A:ILE:HD11	10	0.64	0.09	0.62
(1,137)	1:45:A:ILE:HG13	1:69:A:ILE:HD13	10	0.64	0.09	0.62
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB3	10	0.64	0.02	0.65
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB1	10	0.64	0.02	0.65
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB2	10	0.64	0.02	0.65
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD21	10	0.63	0.88	0.34
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD23	10	0.63	0.88	0.34
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD22	10	0.63	0.88	0.34
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	10	0.63	0.05	0.62
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG23	10	0.63	0.01	0.63

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG22	10	0.63	0.01	0.63
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB1	10	0.63	0.57	0.2
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB3	10	0.63	0.57	0.2
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB2	10	0.63	0.57	0.2
(1,77)	1:94:A:SER:HB2	1:98:A:GLU:HB2	10	0.62	0.26	0.62
(1,77)	1:94:A:SER:HB3	1:98:A:GLU:HB2	10	0.62	0.26	0.62
(1,77)	1:94:A:SER:HB3	1:95:A:VAL:HB	10	0.62	0.26	0.62
(2,1016)	1:34:A:VAL:HG12	1:45:A:ILE:HG23	10	0.62	0.13	0.58
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG22	10	0.62	0.13	0.58
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG21	10	0.62	0.13	0.58
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG23	10	0.62	0.13	0.58
(2,1016)	1:34:A:VAL:HG12	1:45:A:ILE:HG22	10	0.62	0.13	0.58
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB2	10	0.62	0.09	0.62
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB3	10	0.62	0.09	0.62
(2,803)	1:62:A:VAL:HG13	1:76:A:ALA:HB2	10	0.62	0.09	0.62
(2,803)	1:62:A:VAL:HG13	1:76:A:ALA:HB1	10	0.62	0.09	0.62
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB1	10	0.62	0.09	0.62
(2,803)	1:62:A:VAL:HG12	1:76:A:ALA:HB2	10	0.62	0.09	0.62
(1,205)	1:65:A:ILE:HD12	1:62:A:VAL:HG21	10	0.6	0.1	0.56
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG21	10	0.6	0.1	0.56
(1,205)	1:65:A:ILE:HD12	1:62:A:VAL:HG22	10	0.6	0.1	0.56
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG22	10	0.6	0.1	0.56
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG23	10	0.6	0.1	0.56
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	10	0.6	0.06	0.57
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD11	10	0.6	0.06	0.57
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD13	10	0.6	0.06	0.57
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	10	0.59	0.04	0.58
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG22	10	0.59	0.04	0.58
(2,1032)	1:77:A:ILE:HG22	1:77:A:ILE:HD11	10	0.59	0.03	0.58
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD11	10	0.59	0.03	0.58
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD12	10	0.59	0.03	0.58
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD13	10	0.59	0.03	0.58
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG22	10	0.58	0.08	0.56
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG21	10	0.58	0.08	0.56
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG13	10	0.58	0.08	0.56
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG11	10	0.58	0.08	0.56
(2,1012)	1:22:A:ILE:HG21	1:25:A:LYS:HD2	10	0.57	0.07	0.58
(2,1012)	1:22:A:ILE:HG23	1:25:A:LYS:HD2	10	0.57	0.07	0.58
(2,1012)	1:22:A:ILE:HG23	1:25:A:LYS:HD3	10	0.57	0.07	0.58
(2,1012)	1:22:A:ILE:HG22	1:25:A:LYS:HD2	10	0.57	0.07	0.58
(2,875)	1:92:A:MET:HE2	1:61:A:PHE:HB3	10	0.57	0.17	0.64
(2,875)	1:92:A:MET:HE3	1:61:A:PHE:HB3	10	0.57	0.17	0.64

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,875)	1:92:A:MET:HE1	1:61:A:PHE:HB3	10	0.57	0.17	0.64
(1,200)	1:42:A:ILE:HG23	1:69:A:ILE:HD12	10	0.57	0.13	0.6
(1,200)	1:42:A:ILE:HG22	1:69:A:ILE:HD12	10	0.57	0.13	0.6
(1,200)	1:42:A:ILE:HG21	1:69:A:ILE:HD12	10	0.57	0.13	0.6
(1,200)	1:42:A:ILE:HG23	1:69:A:ILE:HD11	10	0.57	0.13	0.6
(1,200)	1:42:A:ILE:HG22	1:69:A:ILE:HD13	10	0.57	0.13	0.6
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB3	10	0.56	0.06	0.57
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB2	10	0.56	0.06	0.57
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB1	10	0.56	0.06	0.57
(2,766)	1:52:A:VAL:HG22	1:52:A:VAL:HA	10	0.55	0.04	0.57
(2,766)	1:52:A:VAL:HG21	1:52:A:VAL:HA	10	0.55	0.04	0.57
(2,766)	1:52:A:VAL:HG23	1:52:A:VAL:HA	10	0.55	0.04	0.57
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG13	10	0.55	0.05	0.54
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG12	10	0.55	0.05	0.54
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG11	10	0.55	0.05	0.54
(2,994)	1:81:A:VAL:HG21	1:81:A:VAL:HG23	10	0.55	0.0	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	10	0.55	0.0	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG23	10	0.55	0.0	0.55
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	10	0.55	0.22	0.69
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG22	10	0.55	0.09	0.55
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	10	0.55	0.09	0.55
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG21	10	0.55	0.09	0.55
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	10	0.55	0.01	0.55
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	10	0.54	0.04	0.53
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG22	10	0.54	0.04	0.53
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG23	10	0.54	0.04	0.53
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG22	10	0.54	0.1	0.5
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG21	10	0.54	0.1	0.5
(1,190)	1:69:A:ILE:HG21	1:45:A:ILE:HG23	10	0.54	0.1	0.5
(1,190)	1:69:A:ILE:HG21	1:45:A:ILE:HG22	10	0.54	0.1	0.5
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG22	10	0.54	0.11	0.56
(2,805)	1:44:A:THR:HG23	1:45:A:ILE:HG21	10	0.54	0.11	0.56
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG23	10	0.54	0.11	0.56
(2,805)	1:44:A:THR:HG22	1:45:A:ILE:HG21	10	0.54	0.11	0.56
(2,805)	1:44:A:THR:HG22	1:45:A:ILE:HG22	10	0.54	0.11	0.56
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG23	10	0.54	0.13	0.54
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG22	10	0.54	0.13	0.54
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG21	10	0.54	0.13	0.54
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	10	0.53	0.02	0.52
(1,189)	1:79:A:ILE:HG23	1:108:A:VAL:HG12	10	0.53	0.02	0.52
(1,189)	1:79:A:ILE:HG23	1:108:A:VAL:HG13	10	0.53	0.02	0.52
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG13	10	0.53	0.02	0.52

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG12	10	0.53	0.02	0.52
(1,181)	1:22:A:ILE:HG22	1:29:A:ARG:HG3	10	0.51	0.19	0.44
(1,181)	1:22:A:ILE:HG21	1:29:A:ARG:HG3	10	0.51	0.19	0.44
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	10	0.51	0.01	0.51
(1,206)	1:65:A:ILE:HD13	1:34:A:VAL:HG21	10	0.51	0.21	0.44
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG21	10	0.51	0.21	0.44
(1,206)	1:65:A:ILE:HD13	1:34:A:VAL:HG22	10	0.51	0.21	0.44
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG23	10	0.51	0.21	0.44
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG22	10	0.51	0.21	0.44
(1,206)	1:65:A:ILE:HD13	1:45:A:ILE:HD12	10	0.51	0.21	0.44
(2,873)	1:22:A:ILE:HD13	1:31:A:PRO:HD2	10	0.51	0.15	0.42
(2,873)	1:22:A:ILE:HD11	1:31:A:PRO:HD2	10	0.51	0.15	0.42
(2,873)	1:22:A:ILE:HD12	1:31:A:PRO:HD2	10	0.51	0.15	0.42
(2,843)	1:17:A:ALA:HB3	1:18:A:GLU:HB2	10	0.51	0.05	0.5
(2,843)	1:17:A:ALA:HB2	1:18:A:GLU:HB2	10	0.51	0.05	0.5
(2,843)	1:17:A:ALA:HB1	1:18:A:GLU:HB2	10	0.51	0.05	0.5
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	10	0.5	0.08	0.5
(2,541)	1:70:A:LYS:HE3	1:43:A:PRO:HA	10	0.5	0.08	0.5
(1,150)	1:71:A:LEU:HD13	1:42:A:ILE:HG13	10	0.49	0.91	0.19
(1,150)	1:71:A:LEU:HD12	1:42:A:ILE:HG13	10	0.49	0.91	0.19
(1,150)	1:71:A:LEU:HD11	1:42:A:ILE:HG13	10	0.49	0.91	0.19
(1,235)	1:73:A:ALA:HB2	1:73:A:ALA:HB1	10	0.49	0.0	0.49
(1,235)	1:73:A:ALA:HB2	1:73:A:ALA:HB3	10	0.49	0.0	0.49
(1,235)	1:88:A:ALA:HB1	1:88:A:ALA:HB3	10	0.49	0.0	0.49
(1,235)	1:88:A:ALA:HB2	1:88:A:ALA:HB3	10	0.49	0.0	0.49
(1,235)	1:88:A:ALA:HB2	1:88:A:ALA:HB1	10	0.49	0.0	0.49
(2,783)	1:109:A:THR:HG21	1:35:A:GLU:HB3	10	0.49	0.44	0.24
(2,783)	1:109:A:THR:HG22	1:35:A:GLU:HB3	10	0.49	0.44	0.24
(2,783)	1:109:A:THR:HG23	1:35:A:GLU:HB3	10	0.49	0.44	0.24
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD22	10	0.49	0.22	0.36
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD23	10	0.49	0.22	0.36
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD21	10	0.49	0.22	0.36
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB2	10	0.48	0.11	0.5
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB3	10	0.48	0.11	0.5
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG13	10	0.48	0.09	0.48
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG11	10	0.48	0.09	0.48
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG12	10	0.48	0.09	0.48
(1,17)	1:35:A:GLU:H	1:108:A:VAL:HB	10	0.48	0.06	0.48
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	10	0.48	0.06	0.48
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD11	10	0.48	0.26	0.42
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD12	10	0.48	0.26	0.42
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD13	10	0.48	0.26	0.42

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG23	10	0.47	0.46	0.27
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG21	10	0.47	0.46	0.27
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG22	10	0.47	0.46	0.27
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	10	0.47	0.09	0.5
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD12	10	0.47	0.09	0.5
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD11	10	0.47	0.09	0.5
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD13	10	0.47	0.07	0.44
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD11	10	0.47	0.07	0.44
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD21	10	0.47	0.07	0.44
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD12	10	0.47	0.07	0.44
(2,738)	1:71:A:LEU:HD12	1:77:A:ILE:HG21	10	0.47	0.42	0.32
(2,738)	1:71:A:LEU:HD11	1:77:A:ILE:HG23	10	0.47	0.42	0.32
(2,738)	1:71:A:LEU:HD13	1:77:A:ILE:HG23	10	0.47	0.42	0.32
(2,738)	1:71:A:LEU:HD12	1:77:A:ILE:HG23	10	0.47	0.42	0.32
(2,738)	1:71:A:LEU:HD13	1:77:A:ILE:HG21	10	0.47	0.42	0.32
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	10	0.47	0.3	0.36
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG22	10	0.47	0.3	0.36
(1,110)	1:110:A:TYR:HB2	1:34:A:VAL:HG21	10	0.47	0.3	0.36
(1,179)	1:22:A:ILE:HG22	1:31:A:PRO:HG3	10	0.46	0.17	0.44
(1,179)	1:22:A:ILE:HG21	1:31:A:PRO:HG3	10	0.46	0.17	0.44
(1,179)	1:22:A:ILE:HG23	1:31:A:PRO:HG3	10	0.46	0.17	0.44
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE3	10	0.46	0.06	0.44
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE1	10	0.46	0.06	0.44
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE2	10	0.46	0.06	0.44
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB2	10	0.46	0.04	0.46
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB1	10	0.46	0.04	0.46
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB3	10	0.46	0.04	0.46
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD11	10	0.46	0.02	0.46
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD12	10	0.46	0.02	0.46
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD13	10	0.46	0.02	0.46
(2,868)	1:92:A:MET:HE2	1:61:A:PHE:HE1	10	0.46	0.13	0.41
(2,868)	1:92:A:MET:HE2	1:61:A:PHE:HE2	10	0.46	0.13	0.41
(2,868)	1:92:A:MET:HE1	1:61:A:PHE:HE2	10	0.46	0.13	0.41
(2,868)	1:92:A:MET:HE3	1:61:A:PHE:HE1	10	0.46	0.13	0.41
(2,868)	1:92:A:MET:HE3	1:61:A:PHE:HE2	10	0.46	0.13	0.41
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	10	0.45	0.17	0.46
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	10	0.44	0.01	0.44
(2,823)	1:76:A:ALA:HB2	1:77:A:ILE:HG23	10	0.44	0.17	0.48
(2,823)	1:76:A:ALA:HB3	1:77:A:ILE:HG23	10	0.44	0.17	0.48
(2,823)	1:76:A:ALA:HB2	1:77:A:ILE:HG22	10	0.44	0.17	0.48
(2,823)	1:76:A:ALA:HB1	1:77:A:ILE:HG22	10	0.44	0.17	0.48
(2,823)	1:76:A:ALA:HB3	1:77:A:ILE:HG22	10	0.44	0.17	0.48

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB1	10	0.44	0.09	0.4
(2,858)	1:20:A:ALA:HB2	1:19:A:ALA:HB2	10	0.44	0.09	0.4
(2,858)	1:20:A:ALA:HB1	1:19:A:ALA:HB1	10	0.44	0.09	0.4
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB2	10	0.44	0.09	0.4
(2,858)	1:20:A:ALA:HB2	1:19:A:ALA:HB1	10	0.44	0.09	0.4
(2,799)	1:108:A:VAL:HG12	1:92:A:MET:HE2	10	0.44	0.12	0.48
(2,799)	1:108:A:VAL:HG13	1:92:A:MET:HE2	10	0.44	0.12	0.48
(2,799)	1:108:A:VAL:HG12	1:92:A:MET:HE3	10	0.44	0.12	0.48
(2,799)	1:108:A:VAL:HG11	1:92:A:MET:HE2	10	0.44	0.12	0.48
(2,799)	1:108:A:VAL:HG11	1:92:A:MET:HE1	10	0.44	0.12	0.48
(2,799)	1:108:A:VAL:HG13	1:92:A:MET:HE1	10	0.44	0.12	0.48
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD12	10	0.44	0.06	0.42
(1,208)	1:93:A:SER:H	1:30:A:ILE:HD12	10	0.44	0.06	0.42
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD11	10	0.44	0.06	0.42
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD13	10	0.44	0.06	0.42
(1,208)	1:93:A:SER:H	1:30:A:ILE:HD13	10	0.44	0.06	0.42
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG13	10	0.44	0.04	0.44
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG11	10	0.44	0.04	0.44
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG12	10	0.44	0.04	0.44
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD11	10	0.44	0.04	0.42
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD12	10	0.44	0.04	0.42
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD13	10	0.44	0.04	0.42
(2,971)	1:57:A:THR:HG22	1:91:A:LEU:HD11	10	0.44	0.04	0.42
(2,971)	1:57:A:THR:HG23	1:91:A:LEU:HD13	10	0.44	0.04	0.42
(2,884)	1:22:A:ILE:HD11	1:31:A:PRO:HB3	10	0.44	0.04	0.44
(2,884)	1:22:A:ILE:HD12	1:31:A:PRO:HB3	10	0.44	0.04	0.44
(2,884)	1:22:A:ILE:HD13	1:31:A:PRO:HB3	10	0.44	0.04	0.44
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD12	10	0.43	0.08	0.4
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	10	0.43	0.08	0.4
(1,62)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	10	0.43	0.08	0.4
(1,227)	1:32:A:VAL:HG11	1:32:A:VAL:HG13	10	0.43	0.0	0.43
(1,227)	1:32:A:VAL:HG12	1:32:A:VAL:HG11	10	0.43	0.0	0.43
(1,227)	1:34:A:VAL:HG11	1:34:A:VAL:HG13	10	0.43	0.0	0.43
(1,227)	1:32:A:VAL:HG12	1:32:A:VAL:HG13	10	0.43	0.0	0.43
(2,940)	1:85:A:LEU:HD21	1:85:A:LEU:HD23	10	0.43	0.0	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD23	10	0.43	0.0	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD21	10	0.43	0.0	0.43
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	10	0.43	0.08	0.41
(1,231)	1:57:A:THR:HG21	1:60:A:GLN:HB2	10	0.43	0.08	0.41
(1,231)	1:57:A:THR:HG22	1:60:A:GLN:HB2	10	0.43	0.08	0.41
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG23	10	0.42	0.1	0.39
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG22	10	0.42	0.1	0.39

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,914)	1:92:A:MET:HE1	1:30:A:ILE:HD11	10	0.42	0.04	0.42
(2,914)	1:92:A:MET:HE3	1:30:A:ILE:HD11	10	0.42	0.04	0.42
(2,914)	1:92:A:MET:HE2	1:30:A:ILE:HD11	10	0.42	0.04	0.42
(2,914)	1:92:A:MET:HE1	1:30:A:ILE:HD13	10	0.42	0.04	0.42
(2,914)	1:92:A:MET:HE2	1:30:A:ILE:HD12	10	0.42	0.04	0.42
(2,914)	1:92:A:MET:HE3	1:30:A:ILE:HD12	10	0.42	0.04	0.42
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG23	10	0.42	0.03	0.42
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG21	10	0.42	0.03	0.42
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG22	10	0.42	0.03	0.42
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	10	0.42	0.1	0.41
(1,209)	1:30:A:ILE:HD11	1:106:A:LEU:HB2	10	0.42	0.1	0.41
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	10	0.42	0.03	0.43
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	10	0.42	0.07	0.44
(2,113)	1:92:A:MET:H	1:57:A:THR:HG22	10	0.42	0.07	0.44
(2,113)	1:92:A:MET:H	1:57:A:THR:HG23	10	0.42	0.07	0.44
(2,1037)	1:92:A:MET:HE1	1:92:A:MET:HE3	10	0.41	0.0	0.41
(2,1037)	1:92:A:MET:HE2	1:92:A:MET:HE3	10	0.41	0.0	0.41
(2,1037)	1:92:A:MET:HE2	1:92:A:MET:HE1	10	0.41	0.0	0.41
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD11	10	0.41	0.1	0.46
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD12	10	0.41	0.1	0.46
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD13	10	0.41	0.1	0.46
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	10	0.41	0.04	0.42
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	10	0.4	0.05	0.42
(2,716)	1:62:A:VAL:HG23	1:59:A:GLY:HA3	10	0.4	0.01	0.4
(2,716)	1:62:A:VAL:HG21	1:59:A:GLY:HA3	10	0.4	0.01	0.4
(2,716)	1:62:A:VAL:HG22	1:59:A:GLY:HA3	10	0.4	0.01	0.4
(2,975)	1:58:A:VAL:HG13	1:92:A:MET:HG2	10	0.4	0.09	0.36
(2,975)	1:58:A:VAL:HG12	1:92:A:MET:HG2	10	0.4	0.09	0.36
(2,975)	1:58:A:VAL:HG11	1:92:A:MET:HG2	10	0.4	0.09	0.36
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG23	10	0.4	0.13	0.4
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG22	10	0.4	0.13	0.4
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG21	10	0.4	0.13	0.4
(1,182)	1:30:A:ILE:HG22	1:32:A:VAL:HB	10	0.39	0.32	0.21
(1,182)	1:30:A:ILE:HG23	1:32:A:VAL:HB	10	0.39	0.32	0.21
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	10	0.39	0.06	0.38
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	10	0.39	0.04	0.39
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG22	10	0.38	0.07	0.42
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG23	10	0.38	0.07	0.42
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG21	10	0.38	0.07	0.42
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG23	10	0.38	0.0	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG22	10	0.38	0.0	0.38
(2,972)	1:109:A:THR:HG22	1:109:A:THR:HG23	10	0.38	0.0	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB2	10	0.38	0.01	0.38
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB3	10	0.38	0.01	0.38
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB1	10	0.38	0.01	0.38
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD12	10	0.37	0.02	0.37
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD11	10	0.37	0.02	0.37
(2,848)	1:73:A:ALA:HB3	1:74:A:GLU:HB3	10	0.37	0.08	0.33
(2,848)	1:73:A:ALA:HB1	1:74:A:GLU:HB3	10	0.37	0.08	0.33
(2,848)	1:73:A:ALA:HB2	1:74:A:GLU:HB3	10	0.37	0.08	0.33
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	10	0.37	0.12	0.4
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB3	10	0.37	0.12	0.4
(2,939)	1:85:A:LEU:HD21	1:85:A:LEU:HD12	10	0.37	0.05	0.38
(2,939)	1:85:A:LEU:HD21	1:85:A:LEU:HD11	10	0.37	0.05	0.38
(2,939)	1:85:A:LEU:HD21	1:85:A:LEU:HD13	10	0.37	0.05	0.38
(2,939)	1:85:A:LEU:HD23	1:85:A:LEU:HD11	10	0.37	0.05	0.38
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD13	10	0.37	0.05	0.38
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD11	10	0.37	0.05	0.38
(2,939)	1:85:A:LEU:HD23	1:85:A:LEU:HD13	10	0.37	0.05	0.38
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD12	10	0.37	0.05	0.38
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB2	10	0.37	0.02	0.38
(2,1001)	1:58:A:VAL:HG13	1:88:A:ALA:HB3	10	0.37	0.02	0.38
(2,1001)	1:58:A:VAL:HG12	1:88:A:ALA:HB1	10	0.37	0.02	0.38
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB3	10	0.37	0.02	0.38
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB1	10	0.37	0.02	0.38
(2,1001)	1:58:A:VAL:HG12	1:88:A:ALA:HB2	10	0.37	0.02	0.38
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	10	0.37	0.08	0.39
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB3	10	0.36	0.0	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB1	10	0.36	0.0	0.36
(2,1002)	1:17:A:ALA:HB1	1:17:A:ALA:HB3	10	0.36	0.0	0.36
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG11	10	0.36	0.03	0.36
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG13	10	0.36	0.03	0.36
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG12	10	0.36	0.03	0.36
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG21	10	0.36	0.09	0.36
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG22	10	0.36	0.09	0.36
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG23	10	0.36	0.09	0.36
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG23	10	0.36	0.14	0.34
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG22	10	0.36	0.14	0.34
(2,938)	1:71:A:LEU:HD13	1:115:A:THR:HG21	10	0.36	0.14	0.34
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG21	10	0.36	0.14	0.34
(2,938)	1:71:A:LEU:HD12	1:115:A:THR:HG21	10	0.36	0.14	0.34
(2,938)	1:71:A:LEU:HD13	1:115:A:THR:HG23	10	0.36	0.14	0.34
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	10	0.36	0.45	0.21
(2,793)	1:57:A:THR:HG21	1:56:A:LEU:HB2	10	0.36	0.45	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,793)	1:57:A:THR:HG22	1:56:A:LEU:HB2	10	0.36	0.45	0.21
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	10	0.36	0.04	0.36
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG22	10	0.36	0.04	0.36
(1,148)	1:51:A:LEU:HD22	1:105:A:PHE:HE2	10	0.35	0.05	0.34
(1,148)	1:51:A:LEU:HD21	1:105:A:PHE:HE2	10	0.35	0.05	0.34
(1,148)	1:51:A:LEU:HD23	1:105:A:PHE:HE2	10	0.35	0.05	0.34
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG11	10	0.35	0.0	0.35
(2,981)	1:108:A:VAL:HG11	1:108:A:VAL:HG13	10	0.35	0.0	0.35
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG13	10	0.35	0.0	0.35
(1,154)	1:109:A:THR:HG21	1:37:A:ALA:H	10	0.35	0.11	0.36
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG22	10	0.35	0.11	0.36
(1,154)	1:109:A:THR:HG22	1:37:A:ALA:H	10	0.35	0.11	0.36
(1,154)	1:109:A:THR:HG23	1:37:A:ALA:H	10	0.35	0.11	0.36
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG21	10	0.35	0.11	0.36
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG23	10	0.35	0.11	0.36
(1,248)	1:50:A:TYR:HE1	1:32:A:VAL:HB	10	0.34	0.17	0.34
(1,248)	1:50:A:TYR:HE1	1:52:A:VAL:HB	10	0.34	0.17	0.34
(1,248)	1:50:A:TYR:HE2	1:32:A:VAL:HB	10	0.34	0.17	0.34
(1,219)	1:3:A:LYS:HD2	1:3:A:LYS:HG3	10	0.34	0.08	0.32
(1,219)	1:3:A:LYS:HD3	1:3:A:LYS:HG2	10	0.34	0.08	0.32
(2,988)	1:76:A:ALA:HB1	1:76:A:ALA:HB3	10	0.34	0.0	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB1	10	0.34	0.0	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB3	10	0.34	0.0	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB3	10	0.34	0.0	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB1	10	0.34	0.0	0.34
(2,1003)	1:20:A:ALA:HB1	1:20:A:ALA:HB3	10	0.34	0.0	0.34
(2,705)	1:62:A:VAL:HG21	1:61:A:PHE:HD1	10	0.33	0.05	0.32
(2,705)	1:62:A:VAL:HG21	1:61:A:PHE:HD2	10	0.33	0.05	0.32
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD2	10	0.33	0.05	0.32
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD1	10	0.33	0.05	0.32
(2,705)	1:62:A:VAL:HG23	1:61:A:PHE:HD2	10	0.33	0.05	0.32
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG22	10	0.33	0.07	0.38
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG23	10	0.33	0.07	0.38
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG21	10	0.33	0.07	0.38
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD12	10	0.33	0.02	0.33
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD11	10	0.33	0.02	0.33
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB1	10	0.33	0.03	0.32
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB2	10	0.33	0.03	0.32
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB3	10	0.33	0.03	0.32
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	10	0.33	0.02	0.33
(2,969)	1:57:A:THR:HG23	1:89:A:GLY:HA2	10	0.33	0.02	0.33
(2,969)	1:57:A:THR:HG21	1:89:A:GLY:HA2	10	0.33	0.02	0.33

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG13	10	0.33	0.0	0.33
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG11	10	0.33	0.0	0.33
(2,984)	1:58:A:VAL:HG11	1:58:A:VAL:HG13	10	0.33	0.0	0.33
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	10	0.33	0.12	0.32
(1,54)	1:111:A:SER:H	1:78:A:PHE:HB2	10	0.33	0.12	0.32
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	10	0.32	0.02	0.32
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG3	10	0.32	0.02	0.32
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	10	0.32	0.07	0.33
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	10	0.32	0.06	0.3
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD11	10	0.32	0.06	0.3
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD13	10	0.32	0.06	0.3
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG22	10	0.32	0.07	0.32
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG21	10	0.32	0.07	0.32
(1,236)	1:37:A:ALA:HB2	1:37:A:ALA:HB3	10	0.32	0.0	0.32
(1,236)	1:54:A:ALA:HB1	1:54:A:ALA:HB3	10	0.32	0.0	0.32
(1,236)	1:54:A:ALA:HB2	1:54:A:ALA:HB3	10	0.32	0.0	0.32
(1,236)	1:54:A:ALA:HB2	1:54:A:ALA:HB1	10	0.32	0.0	0.32
(1,236)	1:37:A:ALA:HB1	1:37:A:ALA:HB3	10	0.32	0.0	0.32
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	10	0.31	0.02	0.32
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB3	10	0.31	0.01	0.31
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB1	10	0.31	0.01	0.31
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB2	10	0.31	0.01	0.31
(2,947)	1:71:A:LEU:HD11	1:71:A:LEU:HD13	10	0.3	0.0	0.3
(2,947)	1:71:A:LEU:HD12	1:71:A:LEU:HD13	10	0.3	0.0	0.3
(2,947)	1:71:A:LEU:HD12	1:71:A:LEU:HD11	10	0.3	0.0	0.3
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB3	10	0.3	0.05	0.3
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB1	10	0.3	0.05	0.3
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB2	10	0.3	0.05	0.3
(2,707)	1:58:A:VAL:HG23	1:57:A:THR:HA	10	0.3	0.04	0.3
(2,707)	1:58:A:VAL:HG21	1:57:A:THR:HA	10	0.3	0.04	0.3
(2,707)	1:58:A:VAL:HG22	1:57:A:THR:HA	10	0.3	0.04	0.3
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD12	10	0.29	0.08	0.26
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD11	10	0.29	0.08	0.26
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD13	10	0.29	0.08	0.26
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	10	0.29	0.12	0.28
(1,19)	1:95:A:VAL:H	1:90:A:ALA:HB1	10	0.29	0.12	0.28
(1,165)	1:32:A:VAL:HG21	1:32:A:VAL:HG11	10	0.29	0.06	0.31
(1,165)	1:32:A:VAL:HG22	1:32:A:VAL:HG12	10	0.29	0.06	0.31
(1,165)	1:32:A:VAL:HG23	1:32:A:VAL:HG13	10	0.29	0.06	0.31
(1,165)	1:52:A:VAL:HG23	1:52:A:VAL:HG11	10	0.29	0.06	0.31
(1,165)	1:52:A:VAL:HG22	1:52:A:VAL:HG12	10	0.29	0.06	0.31
(1,165)	1:52:A:VAL:HG21	1:52:A:VAL:HG11	10	0.29	0.06	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,165)	1:32:A:VAL:HG22	1:32:A:VAL:HG13	10	0.29	0.06	0.31
(1,165)	1:32:A:VAL:HG21	1:32:A:VAL:HG13	10	0.29	0.06	0.31
(2,798)	1:109:A:THR:HG22	1:37:A:ALA:HB2	10	0.29	0.12	0.26
(2,798)	1:109:A:THR:HG23	1:37:A:ALA:HB2	10	0.29	0.12	0.26
(2,798)	1:109:A:THR:HG23	1:37:A:ALA:HB3	10	0.29	0.12	0.26
(2,798)	1:109:A:THR:HG21	1:37:A:ALA:HB2	10	0.29	0.12	0.26
(2,798)	1:109:A:THR:HG21	1:37:A:ALA:HB3	10	0.29	0.12	0.26
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG21	10	0.29	0.03	0.29
(2,1015)	1:79:A:ILE:HG21	1:62:A:VAL:HG22	10	0.29	0.03	0.29
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG22	10	0.29	0.03	0.29
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG23	10	0.29	0.03	0.29
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	10	0.29	0.06	0.3
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG21	10	0.29	0.06	0.3
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG22	10	0.29	0.06	0.3
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD22	10	0.29	0.04	0.28
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD23	10	0.29	0.04	0.28
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD21	10	0.29	0.04	0.28
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	10	0.28	0.02	0.29
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD12	10	0.28	0.04	0.26
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD11	10	0.28	0.04	0.26
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD13	10	0.28	0.04	0.26
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	10	0.28	0.02	0.28
(2,1029)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	10	0.28	0.02	0.28
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	10	0.28	0.02	0.28
(2,1029)	1:62:A:VAL:HG11	1:77:A:ILE:HG22	10	0.28	0.02	0.28
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	10	0.28	0.06	0.27
(2,759)	1:108:A:VAL:HG23	1:108:A:VAL:HA	10	0.28	0.02	0.28
(2,759)	1:108:A:VAL:HG21	1:108:A:VAL:HA	10	0.28	0.02	0.28
(2,759)	1:108:A:VAL:HG22	1:108:A:VAL:HA	10	0.28	0.02	0.28
(2,870)	1:42:A:ILE:HD11	1:67:A:LYS:HA	10	0.27	0.07	0.27
(2,870)	1:42:A:ILE:HD12	1:67:A:LYS:HA	10	0.27	0.07	0.27
(2,870)	1:42:A:ILE:HD13	1:67:A:LYS:HA	10	0.27	0.07	0.27
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG11	10	0.27	0.03	0.27
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG13	10	0.27	0.03	0.27
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG12	10	0.27	0.03	0.27
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	10	0.27	0.05	0.27
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG2	10	0.27	0.1	0.23
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	10	0.27	0.1	0.23
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG12	10	0.26	0.02	0.26
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG11	10	0.26	0.02	0.26
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG13	10	0.26	0.02	0.26
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG22	10	0.26	0.1	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG23	10	0.26	0.1	0.24
(2,973)	1:70:A:LYS:HE2	1:115:A:THR:HG23	10	0.26	0.1	0.24
(2,973)	1:70:A:LYS:HE2	1:115:A:THR:HG22	10	0.26	0.1	0.24
(1,166)	1:34:A:VAL:HG13	1:65:A:ILE:HD13	10	0.26	0.02	0.26
(1,166)	1:34:A:VAL:HG12	1:65:A:ILE:HD12	10	0.26	0.02	0.26
(1,166)	1:34:A:VAL:HG12	1:65:A:ILE:HD13	10	0.26	0.02	0.26
(1,166)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	10	0.26	0.02	0.26
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD12	10	0.26	0.04	0.27
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD11	10	0.26	0.04	0.27
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD13	10	0.26	0.04	0.27
(2,908)	1:77:A:ILE:HD11	1:79:A:ILE:HD12	10	0.26	0.04	0.27
(2,908)	1:77:A:ILE:HD12	1:79:A:ILE:HD11	10	0.26	0.04	0.27
(2,908)	1:77:A:ILE:HD12	1:79:A:ILE:HD12	10	0.26	0.04	0.27
(2,932)	1:113:A:GLU:HG2	1:75:A:LYS:HG3	10	0.26	0.09	0.22
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	10	0.26	0.09	0.22
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG2	10	0.26	0.09	0.22
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	10	0.25	0.02	0.24
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG12	10	0.25	0.02	0.24
(2,959)	1:108:A:VAL:HG23	1:107:A:TYR:HA	10	0.25	0.03	0.26
(2,959)	1:108:A:VAL:HG21	1:107:A:TYR:HA	10	0.25	0.03	0.26
(2,959)	1:108:A:VAL:HG22	1:107:A:TYR:HA	10	0.25	0.03	0.26
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	10	0.25	0.18	0.15
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG3	10	0.25	0.18	0.15
(2,963)	1:62:A:VAL:HG22	1:62:A:VAL:HG23	10	0.25	0.0	0.25
(2,963)	1:62:A:VAL:HG21	1:62:A:VAL:HG23	10	0.25	0.0	0.25
(2,963)	1:62:A:VAL:HG22	1:62:A:VAL:HG21	10	0.25	0.0	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	10	0.25	0.0	0.25
(2,1007)	1:90:A:ALA:HB1	1:90:A:ALA:HB3	10	0.25	0.0	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB1	10	0.25	0.0	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB3	10	0.25	0.0	0.25
(2,1042)	1:79:A:ILE:HD11	1:79:A:ILE:HD13	10	0.25	0.0	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD11	10	0.25	0.0	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD13	10	0.25	0.0	0.25
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG22	10	0.25	0.07	0.23
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG21	10	0.25	0.07	0.23
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG23	10	0.25	0.07	0.23
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	10	0.25	0.09	0.21
(2,671)	1:70:A:LYS:HD3	1:70:A:LYS:HG3	10	0.25	0.09	0.21
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG13	10	0.25	0.05	0.24
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG11	10	0.25	0.05	0.24
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG12	10	0.25	0.05	0.24
(2,982)	1:95:A:VAL:HG22	1:95:A:VAL:HG21	10	0.24	0.0	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,982)	1:95:A:VAL:HG21	1:95:A:VAL:HG23	10	0.24	0.0	0.24
(2,982)	1:95:A:VAL:HG22	1:95:A:VAL:HG23	10	0.24	0.0	0.24
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	10	0.24	0.01	0.24
(2,613)	1:13:A:GLU:HG2	1:13:A:GLU:HB3	10	0.24	0.01	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	10	0.24	0.0	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG21	10	0.24	0.0	0.24
(2,1018)	1:79:A:ILE:HG21	1:79:A:ILE:HG23	10	0.24	0.0	0.24
(2,888)	1:92:A:MET:HE2	1:108:A:VAL:HG21	10	0.24	0.06	0.22
(2,888)	1:92:A:MET:HE2	1:108:A:VAL:HG22	10	0.24	0.06	0.22
(2,888)	1:92:A:MET:HE3	1:108:A:VAL:HG23	10	0.24	0.06	0.22
(2,888)	1:92:A:MET:HE1	1:108:A:VAL:HG23	10	0.24	0.06	0.22
(2,888)	1:92:A:MET:HE3	1:108:A:VAL:HG22	10	0.24	0.06	0.22
(2,888)	1:92:A:MET:HE1	1:108:A:VAL:HG22	10	0.24	0.06	0.22
(2,888)	1:92:A:MET:HE1	1:108:A:VAL:HG21	10	0.24	0.06	0.22
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD3	10	0.23	0.06	0.25
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD2	10	0.23	0.06	0.25
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG12	10	0.23	0.02	0.24
(2,804)	1:64:A:VAL:HG22	1:64:A:VAL:HG11	10	0.23	0.02	0.24
(2,804)	1:64:A:VAL:HG23	1:64:A:VAL:HG13	10	0.23	0.02	0.24
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG13	10	0.23	0.02	0.24
(2,804)	1:64:A:VAL:HG22	1:64:A:VAL:HG12	10	0.23	0.02	0.24
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG11	10	0.23	0.02	0.24
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG11	10	0.23	0.03	0.22
(2,1046)	1:79:A:ILE:HD12	1:108:A:VAL:HG12	10	0.23	0.03	0.22
(2,1046)	1:79:A:ILE:HD11	1:108:A:VAL:HG11	10	0.23	0.03	0.22
(2,1046)	1:79:A:ILE:HD11	1:108:A:VAL:HG13	10	0.23	0.03	0.22
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG13	10	0.23	0.03	0.22
(2,1046)	1:79:A:ILE:HD12	1:108:A:VAL:HG11	10	0.23	0.03	0.22
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG12	10	0.23	0.03	0.22
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	10	0.23	0.04	0.24
(2,931)	1:48:A:LYS:HG3	1:47:A:LYS:HE3	10	0.23	0.04	0.24
(2,931)	1:48:A:LYS:HG3	1:47:A:LYS:HE2	10	0.23	0.04	0.24
(2,990)	1:81:A:VAL:HG22	1:80:A:PHE:HA	10	0.23	0.01	0.23
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	10	0.23	0.01	0.23
(2,990)	1:81:A:VAL:HG21	1:80:A:PHE:HA	10	0.23	0.01	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	10	0.23	0.0	0.23
(2,995)	1:64:A:VAL:HG12	1:64:A:VAL:HG11	10	0.23	0.0	0.23
(2,995)	1:64:A:VAL:HG12	1:64:A:VAL:HG13	10	0.23	0.0	0.23
(1,159)	1:108:A:VAL:HG22	1:34:A:VAL:HA	10	0.22	0.04	0.22
(1,159)	1:108:A:VAL:HG23	1:34:A:VAL:HA	10	0.22	0.04	0.22
(1,159)	1:108:A:VAL:HG21	1:34:A:VAL:HA	10	0.22	0.04	0.22
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	10	0.22	0.01	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,229)	1:32:A:VAL:HG21	1:32:A:VAL:HG23	10	0.22	0.0	0.22
(1,229)	1:52:A:VAL:HG22	1:52:A:VAL:HG23	10	0.22	0.0	0.22
(1,229)	1:52:A:VAL:HG22	1:52:A:VAL:HG21	10	0.22	0.0	0.22
(1,229)	1:52:A:VAL:HG21	1:52:A:VAL:HG23	10	0.22	0.0	0.22
(2,952)	1:51:A:LEU:HD11	1:51:A:LEU:HD13	10	0.22	0.0	0.22
(2,952)	1:51:A:LEU:HD12	1:51:A:LEU:HD11	10	0.22	0.0	0.22
(2,952)	1:51:A:LEU:HD12	1:51:A:LEU:HD13	10	0.22	0.0	0.22
(2,986)	1:62:A:VAL:HG11	1:62:A:VAL:HG13	10	0.22	0.0	0.22
(2,986)	1:62:A:VAL:HG12	1:62:A:VAL:HG13	10	0.22	0.0	0.22
(2,986)	1:62:A:VAL:HG12	1:62:A:VAL:HG11	10	0.22	0.0	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG23	10	0.22	0.0	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	10	0.22	0.0	0.22
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	10	0.22	0.03	0.22
(2,756)	1:57:A:THR:HG22	1:57:A:THR:HA	10	0.22	0.03	0.22
(2,756)	1:57:A:THR:HG23	1:57:A:THR:HA	10	0.22	0.03	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	10	0.22	0.01	0.22
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	10	0.22	0.02	0.22
(2,762)	1:57:A:THR:HG21	1:56:A:LEU:HA	10	0.22	0.02	0.22
(2,762)	1:57:A:THR:HG22	1:56:A:LEU:HA	10	0.22	0.02	0.22
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB2	10	0.21	0.03	0.22
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB1	10	0.21	0.03	0.22
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB3	10	0.21	0.03	0.22
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	10	0.21	0.01	0.21
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG11	10	0.2	0.04	0.18
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG12	10	0.2	0.04	0.18
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG13	10	0.2	0.04	0.18
(2,948)	1:71:A:LEU:HD21	1:71:A:LEU:HD23	10	0.2	0.01	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD23	10	0.2	0.01	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD21	10	0.2	0.01	0.2
(1,172)	1:30:A:ILE:HG22	1:52:A:VAL:H	10	0.2	0.02	0.2
(1,172)	1:30:A:ILE:HG23	1:52:A:VAL:H	10	0.2	0.02	0.2
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	10	0.19	0.05	0.18
(2,554)	1:39:A:LYS:HE3	1:39:A:LYS:HD3	10	0.19	0.05	0.18
(2,554)	1:39:A:LYS:HE3	1:39:A:LYS:HD2	10	0.19	0.05	0.18
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	10	0.19	0.02	0.19
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	10	0.18	0.04	0.17
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB2	10	0.18	0.02	0.18
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB1	10	0.18	0.02	0.18
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB3	10	0.18	0.02	0.18
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	10	0.18	0.04	0.18
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	10	0.18	0.03	0.16
(2,1017)	1:79:A:ILE:HG23	1:108:A:VAL:HG12	10	0.18	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1017)	1:79:A:ILE:HG23	1:108:A:VAL:HG13	10	0.18	0.03	0.16
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG13	10	0.18	0.03	0.16
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG12	10	0.18	0.03	0.16
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD21	10	0.17	0.05	0.18
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD23	10	0.17	0.05	0.18
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD22	10	0.17	0.05	0.18
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD13	10	0.17	0.0	0.17
(2,957)	1:12:A:LEU:HD11	1:12:A:LEU:HD13	10	0.17	0.0	0.17
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD11	10	0.17	0.0	0.17
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	10	0.17	0.02	0.16
(1,68)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	10	0.17	0.02	0.16
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	10	0.17	0.02	0.16
(1,68)	1:62:A:VAL:HG11	1:77:A:ILE:HG22	10	0.17	0.02	0.16
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	10	0.17	0.03	0.16
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG2	10	0.17	0.03	0.16
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	10	0.17	0.0	0.17
(2,819)	1:73:A:ALA:HB3	1:74:A:GLU:HB2	10	0.16	0.01	0.16
(2,819)	1:73:A:ALA:HB1	1:74:A:GLU:HB2	10	0.16	0.01	0.16
(2,819)	1:73:A:ALA:HB2	1:74:A:GLU:HB2	10	0.16	0.01	0.16
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	10	0.16	0.02	0.15
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG23	10	0.16	0.0	0.16
(2,983)	1:108:A:VAL:HG21	1:108:A:VAL:HG23	10	0.16	0.0	0.16
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG21	10	0.16	0.0	0.16
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	10	0.15	0.03	0.14
(2,1050)	1:30:A:ILE:HD11	1:30:A:ILE:HD13	10	0.15	0.0	0.15
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD13	10	0.15	0.0	0.15
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD11	10	0.15	0.0	0.15
(2,791)	1:95:A:VAL:HG23	1:95:A:VAL:HB	10	0.14	0.03	0.14
(2,791)	1:95:A:VAL:HG22	1:95:A:VAL:HB	10	0.14	0.03	0.14
(2,791)	1:95:A:VAL:HG21	1:95:A:VAL:HB	10	0.14	0.03	0.14
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	10	0.13	0.01	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG21	10	0.12	0.0	0.12
(2,1009)	1:42:A:ILE:HG21	1:42:A:ILE:HG23	10	0.12	0.0	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG23	10	0.12	0.0	0.12
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG23	10	0.11	0.0	0.11
(1,239)	1:69:A:ILE:HG21	1:69:A:ILE:HG23	10	0.11	0.0	0.11
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG21	10	0.11	0.0	0.11
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	10	0.1	0.0	0.1
(1,160)	1:12:A:LEU:HD11	1:103:A:ASP:HB3	9	1.02	0.66	1.01
(1,160)	1:12:A:LEU:HD13	1:103:A:ASP:HB3	9	1.02	0.66	1.01
(1,160)	1:12:A:LEU:HD12	1:103:A:ASP:HB3	9	1.02	0.66	1.01
(1,160)	1:12:A:LEU:HD13	1:15:A:ARG:HB2	9	1.02	0.66	1.01

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,780)	1:115:A:THR:HG21	1:116:A:PHE:HB3	9	0.68	0.5	0.54
(2,780)	1:115:A:THR:HG23	1:116:A:PHE:HB3	9	0.68	0.5	0.54
(2,780)	1:115:A:THR:HG22	1:116:A:PHE:HB3	9	0.68	0.5	0.54
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD11	9	0.68	0.1	0.7
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD12	9	0.68	0.1	0.7
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD13	9	0.68	0.1	0.7
(1,226)	1:95:A:VAL:HG11	1:100:A:LYS:HB2	9	0.62	0.14	0.69
(1,226)	1:95:A:VAL:HG11	1:100:A:LYS:HB3	9	0.62	0.14	0.69
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG12	9	0.62	0.14	0.69
(1,226)	1:95:A:VAL:HG12	1:100:A:LYS:HB3	9	0.62	0.14	0.69
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG13	9	0.62	0.14	0.69
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG11	9	0.62	0.14	0.69
(2,711)	1:51:A:LEU:HD21	1:51:A:LEU:HA	9	0.62	0.1	0.65
(2,711)	1:51:A:LEU:HD23	1:51:A:LEU:HA	9	0.62	0.1	0.65
(2,711)	1:51:A:LEU:HD22	1:51:A:LEU:HA	9	0.62	0.1	0.65
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	9	0.53	0.23	0.38
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG21	9	0.5	0.01	0.5
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG23	9	0.5	0.01	0.5
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG22	9	0.5	0.01	0.5
(1,211)	1:33:A:ILE:HD12	1:49:A:LYS:HD3	9	0.47	0.2	0.4
(1,211)	1:33:A:ILE:HD11	1:49:A:LYS:HD2	9	0.47	0.2	0.4
(1,211)	1:33:A:ILE:HD13	1:49:A:LYS:HD3	9	0.47	0.2	0.4
(1,211)	1:33:A:ILE:HD11	1:49:A:LYS:HD3	9	0.47	0.2	0.4
(1,211)	1:33:A:ILE:HD13	1:49:A:LYS:HD2	9	0.47	0.2	0.4
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG22	9	0.44	0.05	0.46
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG21	9	0.44	0.05	0.46
(1,224)	1:51:A:LEU:HD11	1:22:A:ILE:HG21	9	0.44	0.05	0.46
(1,224)	1:51:A:LEU:HD11	1:22:A:ILE:HG23	9	0.44	0.05	0.46
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG23	9	0.44	0.05	0.46
(1,104)	1:47:A:LYS:HE3	1:5:A:SER:HB2	9	0.41	0.27	0.28
(1,104)	1:3:A:LYS:HE3	1:2:A:ALA:HA	9	0.41	0.27	0.28
(1,104)	1:3:A:LYS:HE2	1:5:A:SER:HB2	9	0.41	0.27	0.28
(1,104)	1:3:A:LYS:HE2	1:2:A:ALA:HA	9	0.41	0.27	0.28
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG21	9	0.41	0.16	0.47
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG23	9	0.41	0.16	0.47
(2,699)	1:71:A:LEU:HD12	1:76:A:ALA:H	9	0.4	0.06	0.4
(2,699)	1:71:A:LEU:HD11	1:76:A:ALA:H	9	0.4	0.06	0.4
(2,699)	1:71:A:LEU:HD13	1:76:A:ALA:H	9	0.4	0.06	0.4
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HD2	9	0.39	0.25	0.34
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB3	9	0.39	0.25	0.34
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB2	9	0.39	0.25	0.34
(1,197)	1:45:A:ILE:HG22	1:69:A:ILE:HA	9	0.39	0.14	0.39

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,197)	1:45:A:ILE:HG21	1:69:A:ILE:HA	9	0.39	0.14	0.39
(1,197)	1:45:A:ILE:HG23	1:69:A:ILE:HA	9	0.39	0.14	0.39
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG13	9	0.38	0.2	0.3
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG12	9	0.38	0.2	0.3
(2,753)	1:115:A:THR:HG21	1:116:A:PHE:HD1	9	0.38	0.17	0.32
(2,753)	1:115:A:THR:HG23	1:116:A:PHE:HD1	9	0.38	0.17	0.32
(2,753)	1:115:A:THR:HG22	1:116:A:PHE:HD2	9	0.38	0.17	0.32
(2,753)	1:115:A:THR:HG23	1:116:A:PHE:HD2	9	0.38	0.17	0.32
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD12	9	0.35	0.05	0.34
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD11	9	0.35	0.05	0.34
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD13	9	0.35	0.05	0.34
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	9	0.34	0.18	0.28
(1,105)	1:80:A:PHE:HB2	1:109:A:THR:HB	9	0.34	0.18	0.28
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD23	9	0.33	0.22	0.25
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD22	9	0.33	0.22	0.25
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD21	9	0.33	0.22	0.25
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG22	9	0.31	0.04	0.31
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG21	9	0.31	0.04	0.31
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG23	9	0.31	0.04	0.31
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG13	9	0.3	0.05	0.3
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG12	9	0.3	0.05	0.3
(2,987)	1:77:A:ILE:HD11	1:62:A:VAL:HG11	9	0.3	0.05	0.3
(2,987)	1:77:A:ILE:HD12	1:62:A:VAL:HG13	9	0.3	0.05	0.3
(1,188)	1:54:A:ALA:HB3	1:30:A:ILE:HG13	9	0.26	0.06	0.26
(1,188)	1:54:A:ALA:HB1	1:30:A:ILE:HG13	9	0.26	0.06	0.26
(1,188)	1:54:A:ALA:HB2	1:30:A:ILE:HG13	9	0.26	0.06	0.26
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD13	9	0.26	0.1	0.22
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD11	9	0.26	0.1	0.22
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD12	9	0.26	0.1	0.22
(2,751)	1:64:A:VAL:HG21	1:61:A:PHE:HD2	9	0.26	0.02	0.26
(2,751)	1:64:A:VAL:HG22	1:61:A:PHE:HD1	9	0.26	0.02	0.26
(2,751)	1:64:A:VAL:HG21	1:61:A:PHE:HD1	9	0.26	0.02	0.26
(2,751)	1:64:A:VAL:HG22	1:61:A:PHE:HD2	9	0.26	0.02	0.26
(2,751)	1:64:A:VAL:HG23	1:61:A:PHE:HD1	9	0.26	0.02	0.26
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	9	0.25	0.09	0.25
(1,214)	1:35:A:GLU:HG2	1:5:A:SER:HA	9	0.25	0.09	0.25
(1,169)	1:54:A:ALA:HB3	1:30:A:ILE:HD12	9	0.24	0.05	0.24
(1,169)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	9	0.24	0.05	0.24
(1,169)	1:54:A:ALA:HB2	1:30:A:ILE:HD12	9	0.24	0.05	0.24
(1,169)	1:54:A:ALA:HB3	1:30:A:ILE:HD11	9	0.24	0.05	0.24
(1,169)	1:54:A:ALA:HB1	1:30:A:ILE:HD13	9	0.24	0.05	0.24
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	9	0.24	0.02	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,730)	1:71:A:LEU:HD12	1:67:A:LYS:HB2	9	0.24	0.08	0.28
(2,730)	1:71:A:LEU:HD12	1:67:A:LYS:HB3	9	0.24	0.08	0.28
(2,730)	1:71:A:LEU:HD11	1:67:A:LYS:HB2	9	0.24	0.08	0.28
(2,730)	1:71:A:LEU:HD13	1:67:A:LYS:HB2	9	0.24	0.08	0.28
(2,730)	1:71:A:LEU:HD11	1:67:A:LYS:HB3	9	0.24	0.08	0.28
(2,779)	1:109:A:THR:HG22	1:80:A:PHE:HB2	9	0.24	0.09	0.2
(2,779)	1:109:A:THR:HG23	1:80:A:PHE:HB2	9	0.24	0.09	0.2
(2,779)	1:109:A:THR:HG21	1:80:A:PHE:HB2	9	0.24	0.09	0.2
(1,151)	1:51:A:LEU:HD22	1:22:A:ILE:HD11	9	0.24	0.04	0.23
(1,151)	1:51:A:LEU:HD21	1:22:A:ILE:HD12	9	0.24	0.04	0.23
(1,151)	1:51:A:LEU:HD22	1:22:A:ILE:HD13	9	0.24	0.04	0.23
(1,151)	1:51:A:LEU:HD23	1:22:A:ILE:HD12	9	0.24	0.04	0.23
(2,962)	1:34:A:VAL:HG12	1:45:A:ILE:HG12	9	0.24	0.06	0.22
(2,962)	1:34:A:VAL:HG11	1:45:A:ILE:HG12	9	0.24	0.06	0.22
(2,399)	1:65:A:ILE:HG23	1:77:A:ILE:HD11	9	0.23	0.03	0.22
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD11	9	0.23	0.03	0.22
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD12	9	0.23	0.03	0.22
(2,399)	1:65:A:ILE:HG21	1:77:A:ILE:HD13	9	0.23	0.03	0.22
(2,399)	1:65:A:ILE:HG21	1:77:A:ILE:HD11	9	0.23	0.03	0.22
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD13	9	0.23	0.03	0.22
(2,724)	1:51:A:LEU:HD23	1:29:A:ARG:HB2	9	0.23	0.05	0.22
(2,724)	1:51:A:LEU:HD22	1:29:A:ARG:HB2	9	0.23	0.05	0.22
(2,724)	1:51:A:LEU:HD21	1:29:A:ARG:HB2	9	0.23	0.05	0.22
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	9	0.2	0.09	0.23
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	9	0.19	0.06	0.18
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	9	0.19	0.02	0.19
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB3	9	0.18	0.04	0.19
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB1	9	0.18	0.04	0.19
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB2	9	0.18	0.04	0.19
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG21	9	0.18	0.03	0.17
(2,905)	1:79:A:ILE:HD11	1:62:A:VAL:HG22	9	0.18	0.03	0.17
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG22	9	0.18	0.03	0.17
(2,905)	1:79:A:ILE:HD13	1:62:A:VAL:HG22	9	0.18	0.03	0.17
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG23	9	0.18	0.03	0.17
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	9	0.16	0.03	0.17
(2,901)	1:79:A:ILE:HD13	1:79:A:ILE:HB	9	0.16	0.06	0.13
(2,901)	1:79:A:ILE:HD11	1:79:A:ILE:HB	9	0.16	0.06	0.13
(2,901)	1:79:A:ILE:HD12	1:79:A:ILE:HB	9	0.16	0.06	0.13
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	9	0.16	0.03	0.15
(2,565)	1:39:A:LYS:HE3	1:38:A:GLU:H	9	0.16	0.03	0.15
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	9	0.16	0.04	0.15
(1,78)	1:39:A:LYS:H	1:38:A:GLU:HA	9	0.16	0.04	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,78)	1:12:A:LEU:HA	1:13:A:GLU:H	9	0.16	0.04	0.14
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG23	9	0.15	0.02	0.15
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG22	9	0.15	0.02	0.15
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG21	9	0.15	0.02	0.15
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	9	0.15	0.03	0.14
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG11	9	0.14	0.04	0.13
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG12	9	0.14	0.04	0.13
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG13	9	0.14	0.04	0.13
(1,244)	1:42:A:ILE:HD11	1:69:A:ILE:HD13	9	0.14	0.02	0.13
(1,244)	1:42:A:ILE:HD13	1:69:A:ILE:HD13	9	0.14	0.02	0.13
(1,244)	1:42:A:ILE:HD12	1:69:A:ILE:HD13	9	0.14	0.02	0.13
(1,244)	1:42:A:ILE:HD13	1:69:A:ILE:HD12	9	0.14	0.02	0.13
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	9	0.13	0.02	0.14
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	9	0.13	0.01	0.12
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	9	0.13	0.01	0.13
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG23	9	0.12	0.03	0.12
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG21	9	0.12	0.03	0.12
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG22	9	0.12	0.03	0.12
(2,1035)	1:32:A:VAL:HG21	1:92:A:MET:HE2	8	1.13	1.07	0.5
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE2	8	1.13	1.07	0.5
(2,1035)	1:32:A:VAL:HG23	1:92:A:MET:HE1	8	1.13	1.07	0.5
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE3	8	1.13	1.07	0.5
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE1	8	1.13	1.07	0.5
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	8	0.64	0.06	0.66
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	8	0.55	0.05	0.56
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE3	8	0.55	0.09	0.52
(1,20)	1:109:A:THR:H	1:80:A:PHE:HB2	8	0.55	0.09	0.52
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE2	8	0.55	0.09	0.52
(2,846)	1:33:A:ILE:HG21	1:35:A:GLU:HG3	8	0.51	0.14	0.56
(2,846)	1:33:A:ILE:HG23	1:35:A:GLU:HG3	8	0.51	0.14	0.56
(2,708)	1:85:A:LEU:HD23	1:80:A:PHE:HA	8	0.45	0.69	0.22
(2,708)	1:85:A:LEU:HD22	1:80:A:PHE:HA	8	0.45	0.69	0.22
(2,708)	1:85:A:LEU:HD21	1:80:A:PHE:HA	8	0.45	0.69	0.22
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG21	8	0.38	0.1	0.4
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG23	8	0.38	0.1	0.4
(2,1033)	1:69:A:ILE:HG23	1:65:A:ILE:HG21	8	0.38	0.1	0.4
(2,1033)	1:69:A:ILE:HG23	1:65:A:ILE:HG22	8	0.38	0.1	0.4
(2,872)	1:92:A:MET:HE2	1:61:A:PHE:HB2	8	0.34	0.04	0.34
(2,872)	1:92:A:MET:HE3	1:61:A:PHE:HB2	8	0.34	0.04	0.34
(2,872)	1:92:A:MET:HE1	1:61:A:PHE:HB2	8	0.34	0.04	0.34
(2,1005)	1:88:A:ALA:HB3	1:62:A:VAL:HG22	8	0.33	0.12	0.28
(2,1005)	1:88:A:ALA:HB1	1:62:A:VAL:HG22	8	0.33	0.12	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1005)	1:88:A:ALA:HB2	1:62:A:VAL:HG23	8	0.33	0.12	0.28
(2,1005)	1:88:A:ALA:HB1	1:62:A:VAL:HG23	8	0.33	0.12	0.28
(2,1005)	1:88:A:ALA:HB3	1:62:A:VAL:HG23	8	0.33	0.12	0.28
(2,1005)	1:88:A:ALA:HB3	1:62:A:VAL:HG21	8	0.33	0.12	0.28
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG21	8	0.28	0.1	0.23
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG22	8	0.28	0.1	0.23
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG23	8	0.28	0.1	0.23
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD13	8	0.27	0.1	0.22
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD12	8	0.27	0.1	0.22
(1,139)	1:85:A:LEU:HD11	1:78:A:PHE:HE2	8	0.26	0.07	0.26
(1,139)	1:85:A:LEU:HD13	1:78:A:PHE:HE1	8	0.26	0.07	0.26
(1,139)	1:85:A:LEU:HD12	1:78:A:PHE:HE1	8	0.26	0.07	0.26
(1,139)	1:85:A:LEU:HD12	1:78:A:PHE:HE2	8	0.26	0.07	0.26
(1,178)	1:33:A:ILE:HG22	1:6:A:PHE:HB2	8	0.24	0.14	0.2
(1,178)	1:33:A:ILE:HG21	1:6:A:PHE:HB2	8	0.24	0.14	0.2
(1,178)	1:33:A:ILE:HG21	1:6:A:PHE:HB3	8	0.24	0.14	0.2
(2,978)	1:81:A:VAL:HG11	1:3:A:LYS:HG2	8	0.22	0.05	0.22
(2,978)	1:81:A:VAL:HG12	1:3:A:LYS:HG3	8	0.22	0.05	0.22
(2,978)	1:81:A:VAL:HG11	1:3:A:LYS:HG3	8	0.22	0.05	0.22
(2,978)	1:81:A:VAL:HG12	1:3:A:LYS:HG2	8	0.22	0.05	0.22
(2,978)	1:81:A:VAL:HG13	1:3:A:LYS:HG3	8	0.22	0.05	0.22
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	8	0.21	0.05	0.2
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	8	0.21	0.09	0.2
(2,555)	1:70:A:LYS:HE3	1:42:A:ILE:HG12	8	0.21	0.08	0.18
(2,555)	1:70:A:LYS:HE2	1:42:A:ILE:HG12	8	0.21	0.08	0.18
(2,555)	1:70:A:LYS:HE3	1:42:A:ILE:HG13	8	0.21	0.08	0.18
(2,784)	1:57:A:THR:HG23	1:60:A:GLN:HB2	8	0.2	0.07	0.17
(2,784)	1:57:A:THR:HG21	1:60:A:GLN:HB2	8	0.2	0.07	0.17
(2,784)	1:57:A:THR:HG22	1:60:A:GLN:HB2	8	0.2	0.07	0.17
(1,230)	1:109:A:THR:HG21	1:109:A:THR:HA	8	0.2	0.04	0.19
(1,230)	1:57:A:THR:HG21	1:57:A:THR:HA	8	0.2	0.04	0.19
(1,230)	1:109:A:THR:HG22	1:109:A:THR:HA	8	0.2	0.04	0.19
(1,230)	1:57:A:THR:HG22	1:57:A:THR:HA	8	0.2	0.04	0.19
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	8	0.2	0.02	0.2
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	8	0.2	0.02	0.2
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	8	0.2	0.02	0.2
(2,1048)	1:54:A:ALA:HB3	1:30:A:ILE:HD12	8	0.18	0.03	0.17
(2,1048)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	8	0.18	0.03	0.17
(2,1048)	1:54:A:ALA:HB2	1:30:A:ILE:HD12	8	0.18	0.03	0.17
(2,1048)	1:54:A:ALA:HB3	1:30:A:ILE:HD11	8	0.18	0.03	0.17
(2,1048)	1:54:A:ALA:HB1	1:30:A:ILE:HD13	8	0.18	0.03	0.17
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB1	8	0.16	0.02	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB2	8	0.16	0.02	0.17
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB3	8	0.16	0.02	0.17
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB1	8	0.16	0.02	0.16
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB3	8	0.16	0.02	0.16
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB2	8	0.16	0.02	0.16
(1,127)	1:3:A:LYS:HB3	1:109:A:THR:HB	8	0.15	0.03	0.15
(1,127)	1:3:A:LYS:HB2	1:109:A:THR:HB	8	0.15	0.03	0.15
(2,677)	1:85:A:LEU:HD11	1:78:A:PHE:HD2	8	0.15	0.02	0.15
(2,677)	1:85:A:LEU:HD13	1:78:A:PHE:HD1	8	0.15	0.02	0.15
(2,677)	1:85:A:LEU:HD12	1:78:A:PHE:HD1	8	0.15	0.02	0.15
(2,677)	1:85:A:LEU:HD12	1:78:A:PHE:HD2	8	0.15	0.02	0.15
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD1	8	0.14	0.03	0.14
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD2	8	0.14	0.03	0.14
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB3	8	0.14	0.01	0.14
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB1	8	0.14	0.01	0.14
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	8	0.11	0.01	0.12
(2,727)	1:12:A:LEU:HD21	1:16:A:ARG:HG2	7	0.94	0.65	1.49
(2,727)	1:12:A:LEU:HD22	1:16:A:ARG:HG2	7	0.94	0.65	1.49
(2,727)	1:12:A:LEU:HD23	1:16:A:ARG:HG2	7	0.94	0.65	1.49
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG3	7	0.9	0.32	0.88
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG2	7	0.9	0.32	0.88
(1,158)	1:52:A:VAL:HG23	1:50:A:TYR:HD1	7	0.85	0.16	0.93
(1,158)	1:32:A:VAL:HG22	1:61:A:PHE:HE1	7	0.85	0.16	0.93
(1,158)	1:32:A:VAL:HG21	1:61:A:PHE:HE1	7	0.85	0.16	0.93
(1,158)	1:32:A:VAL:HG21	1:61:A:PHE:HE2	7	0.85	0.16	0.93
(1,158)	1:32:A:VAL:HG23	1:61:A:PHE:HE1	7	0.85	0.16	0.93
(1,158)	1:32:A:VAL:HG23	1:61:A:PHE:HE2	7	0.85	0.16	0.93
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	7	0.81	0.3	0.95
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	7	0.81	0.79	0.17
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG2	7	0.52	0.46	0.21
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG3	7	0.52	0.46	0.21
(1,212)	1:33:A:ILE:HD12	1:49:A:LYS:HG3	7	0.51	0.34	0.29
(1,212)	1:33:A:ILE:HD11	1:49:A:LYS:HG3	7	0.51	0.34	0.29
(1,212)	1:33:A:ILE:HD13	1:49:A:LYS:HG2	7	0.51	0.34	0.29
(1,212)	1:33:A:ILE:HD13	1:49:A:LYS:HG3	7	0.51	0.34	0.29
(1,163)	1:64:A:VAL:HG21	1:52:A:VAL:HB	7	0.46	0.14	0.48
(1,163)	1:57:A:THR:HG21	1:91:A:LEU:HB2	7	0.46	0.14	0.48
(1,163)	1:64:A:VAL:HG22	1:52:A:VAL:HB	7	0.46	0.14	0.48
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	7	0.45	0.31	0.5
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	7	0.44	0.06	0.46
(1,152)	1:109:A:THR:HG22	1:80:A:PHE:H	7	0.4	0.14	0.43
(1,152)	1:109:A:THR:HG23	1:80:A:PHE:H	7	0.4	0.14	0.43

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,152)	1:109:A:THR:HG21	1:80:A:PHE:H	7	0.4	0.14	0.43
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	7	0.36	0.57	0.13
(1,177)	1:79:A:ILE:HG23	1:110:A:TYR:HB2	7	0.32	0.1	0.28
(1,177)	1:79:A:ILE:HG22	1:110:A:TYR:HB2	7	0.32	0.1	0.28
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	7	0.31	0.05	0.31
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	7	0.3	0.04	0.3
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	7	0.28	0.03	0.27
(2,770)	1:115:A:THR:HG23	1:115:A:THR:HA	7	0.24	0.09	0.22
(2,770)	1:115:A:THR:HG22	1:115:A:THR:HA	7	0.24	0.09	0.22
(2,770)	1:115:A:THR:HG21	1:115:A:THR:HA	7	0.24	0.09	0.22
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD21	7	0.2	0.05	0.21
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD22	7	0.2	0.05	0.21
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD23	7	0.2	0.05	0.21
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	7	0.19	0.07	0.18
(2,796)	1:32:A:VAL:HG12	1:32:A:VAL:HB	7	0.17	0.01	0.18
(2,796)	1:32:A:VAL:HG13	1:32:A:VAL:HB	7	0.17	0.01	0.18
(2,796)	1:32:A:VAL:HG11	1:32:A:VAL:HB	7	0.17	0.01	0.18
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	7	0.17	0.03	0.18
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD22	7	0.17	0.05	0.18
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD21	7	0.17	0.05	0.18
(2,731)	1:85:A:LEU:HB3	1:85:A:LEU:HD22	7	0.17	0.05	0.18
(1,201)	1:22:A:ILE:HD11	1:51:A:LEU:HD13	7	0.16	0.03	0.18
(1,201)	1:22:A:ILE:HD13	1:51:A:LEU:HD13	7	0.16	0.03	0.18
(1,201)	1:22:A:ILE:HD13	1:51:A:LEU:HD11	7	0.16	0.03	0.18
(1,201)	1:22:A:ILE:HD12	1:51:A:LEU:HD11	7	0.16	0.03	0.18
(1,201)	1:22:A:ILE:HD12	1:51:A:LEU:HD13	7	0.16	0.03	0.18
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG22	7	0.16	0.07	0.14
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG21	7	0.16	0.07	0.14
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	7	0.14	0.04	0.13
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	7	0.14	0.0	0.14
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	7	0.12	0.01	0.12
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	7	0.12	0.01	0.11
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	7	0.11	0.01	0.11
(1,128)	1:3:A:LYS:HB3	1:35:A:GLU:HB2	6	1.23	1.22	0.97
(1,128)	1:75:A:LYS:HB3	1:74:A:GLU:HB2	6	1.23	1.22	0.97
(2,614)	1:98:A:GLU:HG3	1:97:A:GLU:HG3	6	1.11	0.72	1.42
(2,777)	1:12:A:LEU:HD11	1:103:A:ASP:HB2	6	0.93	0.65	0.87
(2,777)	1:12:A:LEU:HD13	1:103:A:ASP:HB2	6	0.93	0.65	0.87
(2,431)	1:120:A:SER:HB2	1:121:A:PRO:HD2	6	0.78	0.29	0.78
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB1	6	0.48	0.06	0.51
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB2	6	0.48	0.06	0.51
(2,786)	1:12:A:LEU:HD11	1:16:A:ARG:HB2	6	0.36	0.08	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,786)	1:12:A:LEU:HD12	1:16:A:ARG:HB2	6	0.36	0.08	0.38
(2,786)	1:12:A:LEU:HD13	1:16:A:ARG:HB2	6	0.36	0.08	0.38
(2,1054)	1:107:A:TYR:HD1	1:107:A:TYR:HB2	6	0.25	0.1	0.24
(2,869)	1:92:A:MET:HE3	1:58:A:VAL:HA	6	0.24	0.12	0.2
(2,869)	1:92:A:MET:HE1	1:58:A:VAL:HA	6	0.24	0.12	0.2
(2,644)	1:113:A:GLU:H	1:113:A:GLU:HB2	6	0.22	0.04	0.22
(2,1062)	1:50:A:TYR:HE1	1:64:A:VAL:HG12	6	0.22	0.09	0.2
(2,1062)	1:50:A:TYR:HE2	1:64:A:VAL:HG12	6	0.22	0.09	0.2
(2,1062)	1:50:A:TYR:HE1	1:64:A:VAL:HG11	6	0.22	0.09	0.2
(2,1062)	1:50:A:TYR:HE1	1:64:A:VAL:HG13	6	0.22	0.09	0.2
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD11	6	0.2	0.1	0.16
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD12	6	0.2	0.1	0.16
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD13	6	0.2	0.1	0.16
(2,867)	1:92:A:MET:HE3	1:61:A:PHE:HD2	6	0.19	0.05	0.18
(2,867)	1:92:A:MET:HE3	1:61:A:PHE:HD1	6	0.19	0.05	0.18
(2,867)	1:92:A:MET:HE1	1:61:A:PHE:HD2	6	0.19	0.05	0.18
(1,29)	1:109:A:THR:H	1:110:A:TYR:H	6	0.18	0.06	0.22
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG21	6	0.17	0.04	0.17
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG22	6	0.17	0.04	0.17
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG23	6	0.17	0.04	0.17
(2,808)	1:32:A:VAL:HG21	1:32:A:VAL:HG11	6	0.16	0.03	0.16
(2,808)	1:32:A:VAL:HG22	1:32:A:VAL:HG12	6	0.16	0.03	0.16
(2,808)	1:32:A:VAL:HG23	1:32:A:VAL:HG13	6	0.16	0.03	0.16
(2,808)	1:32:A:VAL:HG23	1:32:A:VAL:HG11	6	0.16	0.03	0.16
(2,808)	1:32:A:VAL:HG22	1:32:A:VAL:HG13	6	0.16	0.03	0.16
(2,954)	1:12:A:LEU:HD21	1:12:A:LEU:HD11	6	0.16	0.02	0.16
(2,954)	1:12:A:LEU:HD21	1:12:A:LEU:HD13	6	0.16	0.02	0.16
(2,954)	1:12:A:LEU:HD22	1:12:A:LEU:HD11	6	0.16	0.02	0.16
(2,954)	1:12:A:LEU:HD23	1:12:A:LEU:HD11	6	0.16	0.02	0.16
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG22	6	0.16	0.03	0.15
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG21	6	0.16	0.03	0.15
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG23	6	0.16	0.03	0.15
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG21	6	0.11	0.0	0.11
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG23	6	0.11	0.0	0.11
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG22	6	0.11	0.0	0.11
(2,443)	1:87:A:PRO:HA	1:87:A:PRO:HB2	6	0.1	0.0	0.11
(2,3)	1:37:A:ALA:H	1:36:A:LYS:HB2	5	0.37	0.19	0.43
(2,3)	1:37:A:ALA:H	1:36:A:LYS:HB3	5	0.37	0.19	0.43
(1,146)	1:71:A:LEU:HG	1:77:A:ILE:HG21	5	0.34	0.05	0.33
(1,146)	1:71:A:LEU:HG	1:77:A:ILE:HG23	5	0.34	0.05	0.33
(2,150)	1:47:A:LYS:H	1:45:A:ILE:HG23	5	0.29	0.08	0.27
(2,150)	1:47:A:LYS:H	1:45:A:ILE:HG21	5	0.29	0.08	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB3	5	0.28	0.14	0.24
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB1	5	0.28	0.14	0.24
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB2	5	0.28	0.14	0.24
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG13	5	0.26	0.06	0.24
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG12	5	0.26	0.06	0.24
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG11	5	0.26	0.06	0.24
(2,687)	1:16:A:ARG:HG2	1:16:A:ARG:HB2	5	0.22	0.06	0.24
(2,181)	1:100:A:LYS:H	1:100:A:LYS:HG3	5	0.19	0.06	0.23
(2,181)	1:100:A:LYS:H	1:100:A:LYS:HG2	5	0.19	0.06	0.23
(2,622)	1:75:A:LYS:HB2	1:76:A:ALA:H	5	0.18	0.06	0.16
(3,56)	1:34:A:VAL:N	1:48:A:LYS:O	5	0.14	0.02	0.14
(2,219)	1:49:A:LYS:H	1:48:A:LYS:HB3	5	0.14	0.05	0.12
(1,49)	1:67:A:LYS:H	1:65:A:ILE:H	5	0.14	0.02	0.15
(2,10)	1:85:A:LEU:H	1:80:A:PHE:HD2	5	0.14	0.03	0.13
(2,10)	1:85:A:LEU:H	1:80:A:PHE:HD1	5	0.14	0.03	0.13
(1,48)	1:79:A:ILE:H	1:80:A:PHE:H	5	0.13	0.02	0.12
(2,221)	1:49:A:LYS:H	1:49:A:LYS:HD2	5	0.13	0.02	0.13
(3,43)	1:97:A:GLU:N	1:93:A:SER:O	5	0.12	0.02	0.12
(2,205)	1:62:A:VAL:H	1:59:A:GLY:HA3	5	0.12	0.02	0.11
(2,432)	1:72:A:SER:HB3	1:75:A:LYS:HB3	4	1.46	0.4	1.44
(2,451)	1:94:A:SER:HB3	1:91:A:LEU:HG	4	1.44	0.09	1.45
(2,345)	1:98:A:GLU:H	1:98:A:GLU:HG3	4	0.98	0.15	0.99
(1,69)	1:32:A:VAL:HG22	1:108:A:VAL:HG23	4	0.9	0.59	0.61
(1,69)	1:32:A:VAL:HG23	1:108:A:VAL:HG22	4	0.9	0.59	0.61
(1,69)	1:32:A:VAL:HG23	1:108:A:VAL:HG21	4	0.9	0.59	0.61
(2,170)	1:94:A:SER:H	1:94:A:SER:HB3	4	0.89	0.01	0.89
(2,967)	1:32:A:VAL:HG23	1:108:A:VAL:HG23	4	0.82	0.56	0.72
(2,967)	1:32:A:VAL:HG23	1:108:A:VAL:HG22	4	0.82	0.56	0.72
(2,967)	1:32:A:VAL:HG23	1:108:A:VAL:HG21	4	0.82	0.56	0.72
(2,464)	1:12:A:LEU:HA	1:15:A:ARG:HB3	4	0.82	0.12	0.81
(2,768)	1:12:A:LEU:HA	1:12:A:LEU:HD11	4	0.68	0.32	0.86
(2,768)	1:12:A:LEU:HA	1:12:A:LEU:HD13	4	0.68	0.32	0.86
(2,609)	1:98:A:GLU:HG3	1:98:A:GLU:HA	4	0.62	0.01	0.62
(2,447)	1:94:A:SER:HB3	1:91:A:LEU:HB3	4	0.59	0.05	0.57
(2,930)	1:3:A:LYS:HE3	1:3:A:LYS:HG3	4	0.56	0.44	0.47
(2,930)	1:3:A:LYS:HE2	1:3:A:LYS:HG3	4	0.56	0.44	0.47
(2,324)	1:28:A:ASP:H	1:28:A:ASP:HB2	4	0.5	0.02	0.5
(1,186)	1:30:A:ILE:HG22	1:106:A:LEU:HB2	4	0.46	0.08	0.48
(1,186)	1:30:A:ILE:HG21	1:106:A:LEU:HB3	4	0.46	0.08	0.48
(2,414)	1:111:A:SER:HB3	1:37:A:ALA:HB1	4	0.46	0.12	0.5
(2,414)	1:111:A:SER:HB3	1:37:A:ALA:HB3	4	0.46	0.12	0.5
(2,720)	1:78:A:PHE:HB3	1:85:A:LEU:HD22	4	0.45	0.51	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,720)	1:78:A:PHE:HB3	1:85:A:LEU:HD21	4	0.45	0.51	0.18
(2,483)	1:116:A:PHE:HA	1:116:A:PHE:HD1	4	0.35	0.18	0.36
(2,483)	1:116:A:PHE:HA	1:116:A:PHE:HD2	4	0.35	0.18	0.36
(1,9)	1:108:A:VAL:H	1:107:A:TYR:HE2	4	0.3	0.16	0.28
(1,9)	1:108:A:VAL:H	1:107:A:TYR:HD1	4	0.3	0.16	0.28
(1,3)	1:76:A:ALA:H	1:78:A:PHE:HE1	4	0.24	0.15	0.18
(1,3)	1:76:A:ALA:H	1:78:A:PHE:HE2	4	0.24	0.15	0.18
(1,3)	1:76:A:ALA:H	1:77:A:ILE:H	4	0.24	0.15	0.18
(2,557)	1:39:A:LYS:HE3	1:39:A:LYS:HG2	4	0.22	0.02	0.24
(2,1060)	1:107:A:TYR:HE1	1:3:A:LYS:HE3	4	0.22	0.08	0.23
(2,1060)	1:107:A:TYR:HE1	1:3:A:LYS:HE2	4	0.22	0.08	0.23
(2,882)	1:45:A:ILE:HG21	1:47:A:LYS:HB3	4	0.22	0.08	0.21
(2,882)	1:45:A:ILE:HG23	1:47:A:LYS:HB3	4	0.22	0.08	0.21
(1,153)	1:32:A:VAL:H	1:52:A:VAL:HG23	4	0.2	0.05	0.2
(1,153)	1:32:A:VAL:H	1:32:A:VAL:HG21	4	0.2	0.05	0.2
(1,153)	1:32:A:VAL:H	1:52:A:VAL:HG22	4	0.2	0.05	0.2
(2,487)	1:74:A:GLU:HA	1:74:A:GLU:HG3	4	0.19	0.0	0.19
(2,800)	1:95:A:VAL:HG22	1:90:A:ALA:HB2	4	0.18	0.05	0.16
(2,800)	1:95:A:VAL:HG22	1:90:A:ALA:HB1	4	0.18	0.05	0.16
(2,800)	1:95:A:VAL:HG21	1:90:A:ALA:HB3	4	0.18	0.05	0.16
(2,26)	1:32:A:VAL:H	1:32:A:VAL:HG12	4	0.17	0.03	0.16
(2,26)	1:32:A:VAL:H	1:32:A:VAL:HG13	4	0.17	0.03	0.16
(2,26)	1:32:A:VAL:H	1:32:A:VAL:HG11	4	0.17	0.03	0.16
(1,246)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	4	0.15	0.02	0.16
(1,246)	1:34:A:VAL:HG13	1:65:A:ILE:HD13	4	0.15	0.02	0.16
(2,490)	1:9:A:GLU:HA	1:9:A:GLU:HG3	4	0.15	0.02	0.15
(3,51)	1:33:A:ILE:N	1:106:A:LEU:O	4	0.14	0.04	0.13
(2,176)	1:17:A:ALA:H	1:16:A:ARG:HB3	4	0.14	0.04	0.12
(2,463)	1:60:A:GLN:HA	1:60:A:GLN:HG2	4	0.12	0.01	0.12
(2,121)	1:14:A:LYS:H	1:13:A:GLU:H	4	0.11	0.01	0.11
(2,50)	1:108:A:VAL:H	1:109:A:THR:H	4	0.11	0.01	0.11
(1,7)	1:45:A:ILE:H	1:44:A:THR:HA	4	0.11	0.01	0.11
(2,663)	1:21:A:ARG:HB3	1:22:A:ILE:H	4	0.11	0.0	0.11
(2,1022)	1:32:A:VAL:HG21	1:30:A:ILE:HG23	3	1.79	0.39	1.97
(2,1022)	1:32:A:VAL:HG21	1:30:A:ILE:HG22	3	1.79	0.39	1.97
(2,840)	1:42:A:ILE:HG21	1:40:A:SER:HB2	3	1.24	0.64	1.52
(2,840)	1:42:A:ILE:HG23	1:40:A:SER:HB2	3	1.24	0.64	1.52
(2,745)	1:33:A:ILE:H	1:32:A:VAL:HG12	3	1.22	0.31	1.29
(2,745)	1:33:A:ILE:H	1:32:A:VAL:HG11	3	1.22	0.31	1.29
(2,636)	1:8:A:GLN:HG2	1:9:A:GLU:HB2	3	0.73	0.64	0.38
(2,965)	1:32:A:VAL:HG23	1:32:A:VAL:HA	3	0.61	0.05	0.62
(1,120)	1:113:A:GLU:H	1:113:A:GLU:HG3	3	0.36	0.14	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,74)	1:72:A:SER:HB2	1:75:A:LYS:HG3	3	0.34	0.13	0.26
(1,74)	1:72:A:SER:HB2	1:75:A:LYS:HG2	3	0.34	0.13	0.26
(2,974)	1:115:A:THR:HG21	1:116:A:PHE:HB2	3	0.3	0.22	0.18
(2,974)	1:115:A:THR:HG22	1:116:A:PHE:HB3	3	0.3	0.22	0.18
(2,974)	1:115:A:THR:HG23	1:116:A:PHE:HB3	3	0.3	0.22	0.18
(1,136)	1:29:A:ARG:HG2	1:22:A:ILE:HD11	3	0.3	0.07	0.34
(1,136)	1:29:A:ARG:HG3	1:22:A:ILE:HD13	3	0.3	0.07	0.34
(2,102)	1:11:A:ASP:H	1:12:A:LEU:HA	3	0.3	0.14	0.35
(2,382)	1:55:A:ASP:H	1:55:A:ASP:HB3	3	0.29	0.06	0.33
(1,133)	1:75:A:LYS:HB3	1:71:A:LEU:HD11	3	0.29	0.11	0.36
(1,133)	1:99:A:LYS:HB3	1:95:A:VAL:HG13	3	0.29	0.11	0.36
(1,133)	1:99:A:LYS:HB3	1:95:A:VAL:HG12	3	0.29	0.11	0.36
(2,718)	1:3:A:LYS:HE2	1:3:A:LYS:HG2	3	0.27	0.09	0.3
(2,718)	1:3:A:LYS:HE3	1:3:A:LYS:HG2	3	0.27	0.09	0.3
(2,821)	1:76:A:ALA:HB1	1:67:A:LYS:HB3	3	0.26	0.09	0.32
(2,821)	1:76:A:ALA:HB3	1:67:A:LYS:HB3	3	0.26	0.09	0.32
(2,892)	1:69:A:ILE:HG23	1:69:A:ILE:HD11	3	0.26	0.11	0.24
(2,899)	1:65:A:ILE:HD12	1:61:A:PHE:HE1	3	0.23	0.07	0.23
(2,899)	1:65:A:ILE:HD12	1:61:A:PHE:HE2	3	0.23	0.07	0.23
(1,38)	1:113:A:GLU:H	1:113:A:GLU:HB3	3	0.18	0.04	0.17
(1,156)	1:34:A:VAL:HG11	1:110:A:TYR:H	3	0.16	0.03	0.17
(1,156)	1:34:A:VAL:HG13	1:110:A:TYR:H	3	0.16	0.03	0.17
(1,130)	1:3:A:LYS:HB2	1:3:A:LYS:HG2	3	0.15	0.04	0.13
(1,130)	1:3:A:LYS:HB2	1:3:A:LYS:HG3	3	0.15	0.04	0.13
(2,131)	1:75:A:LYS:H	1:74:A:GLU:HA	3	0.13	0.0	0.13
(2,669)	1:70:A:LYS:HD3	1:70:A:LYS:HB2	3	0.13	0.03	0.12
(2,669)	1:70:A:LYS:HD2	1:70:A:LYS:HB3	3	0.13	0.03	0.12
(2,944)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	3	0.13	0.02	0.13
(2,944)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	3	0.13	0.02	0.13
(3,49)	1:37:A:ALA:N	1:110:A:TYR:O	3	0.13	0.02	0.13
(2,346)	1:99:A:LYS:H	1:98:A:GLU:HB2	3	0.12	0.02	0.12
(2,341)	1:77:A:ILE:H	1:76:A:ALA:HA	3	0.12	0.01	0.11
(3,42)	1:98:A:GLU:H	1:94:A:SER:O	3	0.12	0.0	0.12
(2,484)	1:3:A:LYS:HA	1:109:A:THR:HB	3	0.11	0.01	0.11
(3,1)	1:26:A:TYR:N	1:22:A:ILE:O	3	0.11	0.0	0.11
(2,701)	1:85:A:LEU:HD21	1:79:A:ILE:H	2	1.28	0.96	1.28
(1,223)	1:71:A:LEU:HD13	1:42:A:ILE:HD13	2	1.28	0.94	1.28
(2,623)	1:8:A:GLN:H	1:8:A:GLN:HG2	2	0.58	0.3	0.58
(2,434)	1:72:A:SER:HB3	1:75:A:LYS:HG2	2	0.52	0.1	0.52
(1,15)	1:11:A:ASP:H	1:10:A:HIS:HB3	2	0.48	0.08	0.48
(1,4)	1:76:A:ALA:H	1:75:A:LYS:HB3	2	0.34	0.05	0.34
(2,754)	1:34:A:VAL:HG21	1:50:A:TYR:HE1	2	0.34	0.2	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,754)	1:34:A:VAL:HG22	1:50:A:TYR:HE2	2	0.34	0.2	0.34
(1,157)	1:34:A:VAL:HG22	1:61:A:PHE:HE1	2	0.33	0.02	0.33
(1,157)	1:34:A:VAL:HG21	1:61:A:PHE:HE2	2	0.33	0.02	0.33
(2,764)	1:109:A:THR:HG23	1:37:A:ALA:HA	2	0.32	0.09	0.32
(2,764)	1:109:A:THR:HG21	1:37:A:ALA:HA	2	0.32	0.09	0.32
(1,63)	1:79:A:ILE:HD11	1:62:A:VAL:HG21	2	0.31	0.02	0.31
(1,167)	1:65:A:ILE:HD13	1:34:A:VAL:HG22	2	0.3	0.1	0.3
(1,167)	1:65:A:ILE:HD12	1:34:A:VAL:HG21	2	0.3	0.1	0.3
(1,142)	1:51:A:LEU:HG	1:22:A:ILE:HD13	2	0.29	0.02	0.29
(1,142)	1:51:A:LEU:HG	1:22:A:ILE:HD12	2	0.29	0.02	0.29
(2,440)	1:6:A:PHE:HA	1:6:A:PHE:HD1	2	0.28	0.14	0.28
(2,440)	1:6:A:PHE:HA	1:6:A:PHE:HD2	2	0.28	0.14	0.28
(2,367)	1:40:A:SER:H	1:37:A:ALA:HB2	2	0.26	0.05	0.26
(2,367)	1:40:A:SER:H	1:37:A:ALA:HB1	2	0.26	0.05	0.26
(2,535)	1:78:A:PHE:HB2	1:80:A:PHE:HE2	2	0.25	0.02	0.25
(2,535)	1:78:A:PHE:HB3	1:80:A:PHE:HE1	2	0.25	0.02	0.25
(1,250)	1:107:A:TYR:HE2	1:6:A:PHE:HB3	2	0.21	0.1	0.21
(1,250)	1:107:A:TYR:HE2	1:6:A:PHE:HB2	2	0.21	0.1	0.21
(2,559)	1:3:A:LYS:HE3	1:81:A:VAL:HG11	2	0.2	0.06	0.2
(2,559)	1:3:A:LYS:HE3	1:81:A:VAL:HG12	2	0.2	0.06	0.2
(2,276)	1:70:A:LYS:H	1:44:A:THR:HG22	2	0.2	0.09	0.2
(2,619)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	2	0.2	0.02	0.2
(1,225)	1:32:A:VAL:HG12	1:32:A:VAL:HA	2	0.16	0.01	0.16
(2,726)	1:67:A:LYS:HG2	1:67:A:LYS:HD3	2	0.16	0.02	0.16
(2,209)	1:118:A:PHE:H	1:118:A:PHE:HB3	2	0.15	0.01	0.15
(2,755)	1:109:A:THR:HG22	1:109:A:THR:HA	2	0.15	0.02	0.15
(2,755)	1:109:A:THR:HG23	1:109:A:THR:HA	2	0.15	0.02	0.15
(1,195)	1:42:A:ILE:HD11	1:77:A:ILE:HA	2	0.14	0.03	0.14
(1,195)	1:42:A:ILE:HD13	1:77:A:ILE:HA	2	0.14	0.03	0.14
(2,692)	1:71:A:LEU:HG	1:67:A:LYS:HB2	2	0.14	0.03	0.14
(2,139)	1:116:A:PHE:H	1:116:A:PHE:HB3	2	0.14	0.02	0.14
(2,610)	1:13:A:GLU:HA	1:13:A:GLU:HG2	2	0.14	0.01	0.14
(1,91)	1:88:A:ALA:HA	1:62:A:VAL:HG22	2	0.13	0.0	0.13
(1,91)	1:88:A:ALA:HA	1:62:A:VAL:HG23	2	0.13	0.0	0.13
(1,187)	1:58:A:VAL:HG21	1:90:A:ALA:HB2	2	0.12	0.02	0.12
(1,187)	1:58:A:VAL:HG22	1:90:A:ALA:HB2	2	0.12	0.02	0.12
(3,21)	1:16:A:ARG:N	1:12:A:LEU:O	2	0.12	0.02	0.12
(2,547)	1:70:A:LYS:HE3	1:43:A:PRO:HG2	2	0.12	0.02	0.12
(3,20)	1:17:A:ALA:H	1:13:A:GLU:O	2	0.12	0.0	0.12
(2,253)	1:113:A:GLU:H	1:115:A:THR:HB	2	0.12	0.02	0.12
(2,261)	1:66:A:ARG:H	1:62:A:VAL:HA	2	0.12	0.0	0.12
(2,310)	1:10:A:HIS:H	1:9:A:GLU:HB2	2	0.11	0.0	0.11

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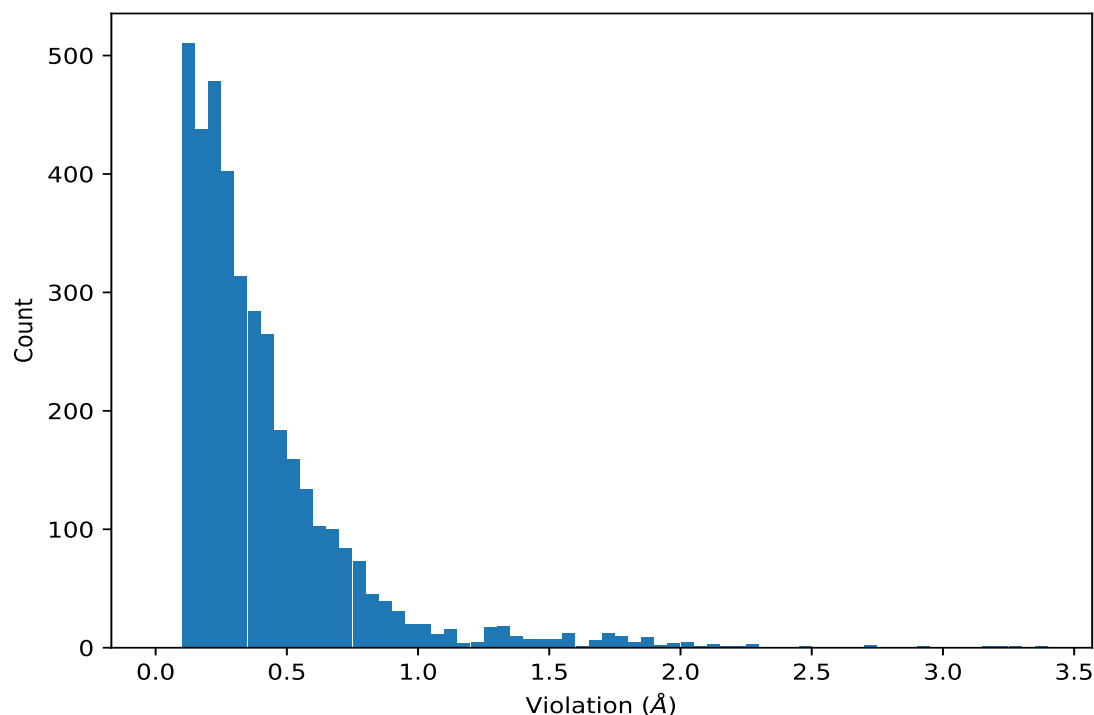
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,567)	1:41:A:ASP:HB3	1:41:A:ASP:HA	2	0.11	0.0	0.11
(3,6)	1:24:A:GLU:H	1:20:A:ALA:O	2	0.11	0.0	0.11
(2,119)	1:109:A:THR:H	1:110:A:TYR:H	2	0.11	0.0	0.11
(2,207)	1:21:A:ARG:H	1:19:A:ALA:HA	2	0.11	0.0	0.11

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:75:A:LYS:HB3	1:74:A:GLU:HB2	4	3.39
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD21	3	3.28
(1,150)	1:71:A:LEU:HD11	1:42:A:ILE:HG13	9	3.23
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG12	2	3.16
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	2	2.91
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE3	7	2.74
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	2	2.72
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE3	8	2.48
(2,708)	1:85:A:LEU:HD23	1:80:A:PHE:HA	3	2.28
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE1	10	2.25
(2,701)	1:85:A:LEU:HD21	1:79:A:ILE:H	3	2.25
(1,223)	1:71:A:LEU:HD13	1:42:A:ILE:HD13	9	2.22
(2,818)	1:54:A:ALA:HB2	1:28:A:ASP:HB3	7	2.15
(2,1022)	1:32:A:VAL:HG21	1:30:A:ILE:HG22	10	2.14
(2,818)	1:54:A:ALA:HB2	1:28:A:ASP:HB3	4	2.13
(2,818)	1:54:A:ALA:HB2	1:28:A:ASP:HB3	2	2.11
(1,162)	1:52:A:VAL:HG23	1:29:A:ARG:HB2	8	2.09
(2,432)	1:72:A:SER:HB3	1:75:A:LYS:HB3	6	2.04
(1,215)	1:35:A:GLU:HG2	1:5:A:SER:HB3	10	2.03
(2,818)	1:54:A:ALA:HB1	1:28:A:ASP:HB3	6	2.02
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	8	2.02
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG12	5	2.0
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG13	6	1.99
(2,1022)	1:32:A:VAL:HG21	1:30:A:ILE:HG23	7	1.97
(2,777)	1:12:A:LEU:HD13	1:103:A:ASP:HB2	9	1.97
(1,162)	1:52:A:VAL:HG21	1:92:A:MET:HB2	10	1.96
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA2	10	1.93
(1,160)	1:12:A:LEU:HD13	1:103:A:ASP:HB3	9	1.92
(1,162)	1:52:A:VAL:HG22	1:92:A:MET:HB2	7	1.89
(1,160)	1:12:A:LEU:HD13	1:103:A:ASP:HB3	3	1.89
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	5	1.89
(1,69)	1:32:A:VAL:HG22	1:108:A:VAL:HG23	8	1.89
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	10	1.88
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	8	1.88
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	9	1.87
(2,840)	1:42:A:ILE:HG21	1:40:A:SER:HB2	3	1.85
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	6	1.85
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	1	1.83
(1,128)	1:75:A:LYS:HB3	1:74:A:GLU:HB2	10	1.82
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	2	1.82
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	7	1.8
(2,614)	1:98:A:GLU:HG3	1:97:A:GLU:HG3	4	1.8
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	5	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,614)	1:98:A:GLU:HG3	1:97:A:GLU:HG3	10	1.79
(1,128)	1:75:A:LYS:HB3	1:74:A:GLU:HB2	5	1.79
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	4	1.76
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	5	1.76
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	6	1.76
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	10	1.76
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	3	1.75
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	9	1.75
(1,42)	1:84:A:VAL:H	1:81:A:VAL:HG22	2	1.75
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	1	1.74
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	2	1.74
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	10	1.74
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	3	1.73
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	8	1.72
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	9	1.72
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	4	1.71
(2,738)	1:71:A:LEU:HD13	1:77:A:ILE:HG21	9	1.7
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	2	1.7
(2,673)	1:45:A:ILE:HG13	1:47:A:LYS:HB3	4	1.7
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	10	1.7
(1,233)	1:84:A:VAL:HG22	1:86:A:PRO:HD2	1	1.7
(2,967)	1:32:A:VAL:HG23	1:108:A:VAL:HG23	8	1.69
(2,775)	1:58:A:VAL:HG13	1:61:A:PHE:HB2	4	1.68
(1,233)	1:84:A:VAL:HG22	1:86:A:PRO:HD2	9	1.68
(1,160)	1:12:A:LEU:HD13	1:103:A:ASP:HB3	6	1.68
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	7	1.65
(2,523)	1:27:A:PRO:HD3	1:22:A:ILE:HA	8	1.65
(2,636)	1:8:A:GLN:HG2	1:9:A:GLU:HB2	10	1.63
(2,783)	1:109:A:THR:HG22	1:35:A:GLU:HB3	8	1.59
(2,852)	1:20:A:ALA:HB3	1:23:A:ARG:HG3	2	1.58
(2,852)	1:20:A:ALA:HB1	1:23:A:ARG:HG3	6	1.58
(2,852)	1:20:A:ALA:HB3	1:23:A:ARG:HG3	9	1.58
(2,17)	1:85:A:LEU:H	1:84:A:VAL:HG21	2	1.57
(2,852)	1:20:A:ALA:HB1	1:23:A:ARG:HG3	5	1.56
(2,775)	1:58:A:VAL:HG13	1:61:A:PHE:HB2	9	1.56
(2,852)	1:20:A:ALA:HB1	1:23:A:ARG:HG3	3	1.55
(2,852)	1:20:A:ALA:HB1	1:23:A:ARG:HG3	7	1.55
(2,852)	1:20:A:ALA:HB3	1:23:A:ARG:HG3	10	1.55
(2,745)	1:33:A:ILE:H	1:32:A:VAL:HG11	10	1.55
(2,451)	1:94:A:SER:HB3	1:91:A:LEU:HG	2	1.55
(2,840)	1:42:A:ILE:HG23	1:40:A:SER:HB2	10	1.52
(2,727)	1:12:A:LEU:HD21	1:16:A:ARG:HG2	5	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,432)	1:72:A:SER:HB3	1:75:A:LYS:HB3	1	1.52
(2,614)	1:98:A:GLU:HG3	1:97:A:GLU:HG3	9	1.51
(2,451)	1:94:A:SER:HB3	1:91:A:LEU:HG	10	1.51
(2,775)	1:58:A:VAL:HG13	1:61:A:PHE:HB2	1	1.5
(2,727)	1:12:A:LEU:HD22	1:16:A:ARG:HG2	7	1.5
(2,775)	1:58:A:VAL:HG11	1:61:A:PHE:HB2	10	1.49
(2,727)	1:12:A:LEU:HD21	1:16:A:ARG:HG2	8	1.49
(2,727)	1:12:A:LEU:HD23	1:16:A:ARG:HG2	10	1.49
(1,228)	1:30:A:ILE:HG13	1:52:A:VAL:HG23	8	1.49
(2,775)	1:58:A:VAL:HG12	1:61:A:PHE:HB2	2	1.48
(2,775)	1:58:A:VAL:HG11	1:61:A:PHE:HB2	6	1.48
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD11	4	1.48
(2,775)	1:58:A:VAL:HG13	1:61:A:PHE:HB2	8	1.44
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB1	2	1.44
(2,780)	1:115:A:THR:HG22	1:116:A:PHE:HB3	10	1.43
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	4	1.43
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG21	6	1.41
(2,775)	1:58:A:VAL:HG13	1:61:A:PHE:HB2	5	1.4
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB3	4	1.4
(2,451)	1:94:A:SER:HB3	1:91:A:LEU:HG	5	1.39
(2,775)	1:58:A:VAL:HG11	1:61:A:PHE:HB2	3	1.38
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	8	1.38
(2,432)	1:72:A:SER:HB3	1:75:A:LYS:HB3	2	1.37
(1,228)	1:30:A:ILE:HG13	1:52:A:VAL:HG22	7	1.37
(2,780)	1:115:A:THR:HG21	1:116:A:PHE:HB3	2	1.36
(2,776)	1:12:A:LEU:HD13	1:16:A:ARG:HD2	6	1.36
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG23	1	1.36
(1,191)	1:65:A:ILE:HG21	1:42:A:ILE:HD11	9	1.36
(2,777)	1:12:A:LEU:HD13	1:103:A:ASP:HB2	3	1.35
(2,775)	1:58:A:VAL:HG13	1:61:A:PHE:HB2	7	1.34
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD12	6	1.34
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD23	3	1.34
(2,949)	1:51:A:LEU:HD13	1:51:A:LEU:HA	10	1.33
(2,720)	1:78:A:PHE:HB3	1:85:A:LEU:HD21	3	1.33
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG2	10	1.33
(2,614)	1:98:A:GLU:HG3	1:97:A:GLU:HG3	3	1.33
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	8	1.33
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	4	1.32
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	5	1.32
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD11	4	1.32
(2,451)	1:94:A:SER:HB3	1:91:A:LEU:HG	6	1.32
(1,228)	1:30:A:ILE:HG13	1:52:A:VAL:HG21	10	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB3	10	1.32
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG2	2	1.32
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	1	1.31
(2,822)	1:76:A:ALA:HB1	1:67:A:LYS:HD3	6	1.3
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	6	1.3
(2,745)	1:33:A:ILE:H	1:32:A:VAL:HG12	7	1.29
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG3	1	1.29
(2,776)	1:12:A:LEU:HD13	1:16:A:ARG:HD3	9	1.28
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	2	1.28
(2,431)	1:120:A:SER:HB2	1:121:A:PRO:HD2	5	1.28
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	2	1.28
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	6	1.28
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	10	1.27
(2,777)	1:12:A:LEU:HD13	1:103:A:ASP:HB2	6	1.26
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	8	1.26
(2,1022)	1:32:A:VAL:HG21	1:30:A:ILE:HG23	8	1.25
(2,776)	1:12:A:LEU:HD13	1:16:A:ARG:HD2	3	1.25
(2,774)	1:57:A:THR:HG22	1:89:A:GLY:HA3	3	1.25
(2,774)	1:57:A:THR:HG21	1:89:A:GLY:HA3	9	1.25
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG23	1	1.25
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG23	9	1.25
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD11	4	1.25
(2,774)	1:57:A:THR:HG23	1:89:A:GLY:HA3	7	1.23
(1,160)	1:12:A:LEU:HD11	1:103:A:ASP:HB3	5	1.23
(1,191)	1:65:A:ILE:HG23	1:45:A:ILE:HG23	10	1.21
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	1	1.21
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	3	1.2
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	4	1.19
(2,930)	1:3:A:LYS:HE2	1:3:A:LYS:HG3	6	1.18
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	3	1.16
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD11	10	1.15
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB2	3	1.14
(2,822)	1:76:A:ALA:HB3	1:67:A:LYS:HD3	9	1.13
(2,345)	1:98:A:GLU:H	1:98:A:GLU:HG3	9	1.13
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	3	1.13
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	9	1.13
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	4	1.13
(2,345)	1:98:A:GLU:H	1:98:A:GLU:HG3	3	1.12
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB3	5	1.12
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	6	1.11
(1,95)	1:90:A:ALA:HA	1:95:A:VAL:HG21	7	1.11
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG23	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	5	1.11
(2,923)	1:5:A:SER:HA	1:8:A:GLN:HB3	4	1.1
(2,822)	1:76:A:ALA:HB2	1:67:A:LYS:HD3	7	1.1
(2,709)	1:85:A:LEU:HD23	1:85:A:LEU:HA	3	1.1
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	1	1.1
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	10	1.09
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	4	1.08
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG21	10	1.08
(2,860)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	10	1.07
(2,822)	1:76:A:ALA:HB2	1:67:A:LYS:HD3	3	1.07
(1,95)	1:90:A:ALA:HA	1:95:A:VAL:HG22	8	1.07
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB2	6	1.07
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	8	1.07
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	9	1.06
(2,780)	1:115:A:THR:HG21	1:116:A:PHE:HB3	1	1.05
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG22	4	1.05
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	2	1.04
(1,182)	1:30:A:ILE:HG23	1:32:A:VAL:HB	8	1.04
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG2	7	1.04
(2,780)	1:115:A:THR:HG22	1:116:A:PHE:HB3	5	1.03
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	5	1.03
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB2	4	1.03
(1,104)	1:47:A:LYS:HE3	1:5:A:SER:HB2	4	1.03
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	2	1.03
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	7	1.02
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	7	1.02
(1,212)	1:33:A:ILE:HD12	1:49:A:LYS:HG3	6	1.02
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	10	1.02
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	7	1.02
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	8	1.01
(1,160)	1:12:A:LEU:HD11	1:103:A:ASP:HB3	8	1.01
(1,158)	1:52:A:VAL:HG23	1:50:A:TYR:HD1	1	1.01
(1,158)	1:32:A:VAL:HG23	1:61:A:PHE:HE2	6	1.01
(1,212)	1:33:A:ILE:HD12	1:49:A:LYS:HG3	2	1.0
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	8	1.0
(1,95)	1:90:A:ALA:HA	1:95:A:VAL:HG21	5	1.0
(2,308)	1:26:A:TYR:H	1:27:A:PRO:HB3	10	0.99
(1,43)	1:66:A:ARG:H	1:77:A:ILE:HG22	10	0.99
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG2	9	0.98
(2,464)	1:12:A:LEU:HA	1:15:A:ARG:HB3	1	0.98
(1,191)	1:65:A:ILE:HG22	1:42:A:ILE:HD13	6	0.98
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	7	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG11	9	0.98
(1,158)	1:32:A:VAL:HG21	1:61:A:PHE:HE1	3	0.97
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG22	6	0.97
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	6	0.96
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD23	10	0.96
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	5	0.96
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	6	0.96
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	7	0.96
(2,898)	1:65:A:ILE:HD11	1:61:A:PHE:HD2	2	0.95
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	3	0.95
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	5	0.95
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	4	0.95
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	6	0.95
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG21	2	0.95
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	7	0.94
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	4	0.94
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	2	0.94
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	5	0.94
(2,898)	1:65:A:ILE:HD12	1:61:A:PHE:HD1	3	0.93
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG21	3	0.93
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG21	4	0.93
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG21	6	0.93
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	5	0.93
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	1	0.93
(2,432)	1:72:A:SER:HB3	1:75:A:LYS:HB3	10	0.93
(1,158)	1:32:A:VAL:HG23	1:61:A:PHE:HE1	5	0.93
(1,77)	1:94:A:SER:HB3	1:98:A:GLU:HB2	8	0.93
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG12	6	0.93
(2,898)	1:65:A:ILE:HD11	1:61:A:PHE:HD1	5	0.92
(2,898)	1:65:A:ILE:HD13	1:61:A:PHE:HD2	6	0.92
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG22	1	0.92
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG22	2	0.92
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG23	8	0.92
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	4	0.92
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG22	5	0.91
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG21	7	0.91
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG23	9	0.91
(2,842)	1:30:A:ILE:HG22	1:96:A:TYR:HB2	8	0.91
(2,822)	1:76:A:ALA:HB1	1:67:A:LYS:HD3	4	0.91
(1,181)	1:22:A:ILE:HG22	1:29:A:ARG:HG3	10	0.91
(1,77)	1:94:A:SER:HB3	1:95:A:VAL:HB	4	0.91
(1,77)	1:94:A:SER:HB3	1:98:A:GLU:HB2	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,852)	1:20:A:ALA:HB1	1:23:A:ARG:HG3	8	0.9
(2,170)	1:94:A:SER:H	1:94:A:SER:HB3	5	0.9
(2,170)	1:94:A:SER:H	1:94:A:SER:HB3	10	0.9
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	10	0.89
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	7	0.89
(1,228)	1:32:A:VAL:HG23	1:106:A:LEU:HD21	1	0.89
(1,179)	1:22:A:ILE:HG22	1:31:A:PRO:HG3	8	0.89
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD11	7	0.89
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	8	0.89
(2,768)	1:12:A:LEU:HA	1:12:A:LEU:HD11	3	0.88
(2,623)	1:8:A:GLN:H	1:8:A:GLN:HG2	10	0.88
(2,464)	1:12:A:LEU:HA	1:15:A:ARG:HB3	7	0.88
(2,170)	1:94:A:SER:H	1:94:A:SER:HB3	2	0.88
(2,170)	1:94:A:SER:H	1:94:A:SER:HB3	6	0.88
(1,228)	1:32:A:VAL:HG21	1:106:A:LEU:HD21	6	0.88
(1,168)	1:62:A:VAL:HG11	1:65:A:ILE:HD11	7	0.88
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG2	8	0.88
(2,898)	1:65:A:ILE:HD12	1:61:A:PHE:HD1	4	0.87
(2,768)	1:12:A:LEU:HA	1:12:A:LEU:HD11	6	0.87
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG22	2	0.87
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG22	3	0.87
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	1	0.87
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD21	9	0.87
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD11	8	0.87
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	4	0.87
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG22	9	0.87
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG12	3	0.87
(2,967)	1:32:A:VAL:HG23	1:108:A:VAL:HG21	7	0.86
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	8	0.86
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	3	0.86
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	9	0.86
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG11	1	0.86
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD12	4	0.85
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	9	0.85
(2,768)	1:12:A:LEU:HA	1:12:A:LEU:HD11	9	0.85
(2,431)	1:120:A:SER:HB2	1:121:A:PRO:HD2	2	0.85
(2,345)	1:98:A:GLU:H	1:98:A:GLU:HG3	4	0.85
(1,206)	1:65:A:ILE:HD13	1:45:A:ILE:HD12	10	0.85
(1,205)	1:65:A:ILE:HD12	1:62:A:VAL:HG22	10	0.85
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	1	0.85
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG23	1	0.85
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG11	2	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG23	8	0.84
(2,898)	1:65:A:ILE:HD12	1:61:A:PHE:HD2	1	0.84
(2,898)	1:65:A:ILE:HD11	1:61:A:PHE:HD1	8	0.84
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD11	10	0.84
(2,860)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	6	0.84
(1,191)	1:65:A:ILE:HG21	1:42:A:ILE:HD13	8	0.84
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB1	1	0.84
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD12	1	0.84
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	7	0.84
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG2	6	0.84
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	10	0.84
(2,898)	1:65:A:ILE:HD11	1:61:A:PHE:HD2	9	0.83
(2,866)	1:65:A:ILE:H	1:65:A:ILE:HG21	10	0.83
(2,822)	1:76:A:ALA:HB3	1:67:A:LYS:HD3	10	0.83
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG21	7	0.83
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	3	0.83
(1,182)	1:30:A:ILE:HG23	1:32:A:VAL:HB	7	0.83
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	3	0.83
(1,77)	1:94:A:SER:HB3	1:98:A:GLU:HB2	5	0.83
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD12	1	0.82
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	8	0.82
(2,783)	1:109:A:THR:HG21	1:35:A:GLU:HB3	1	0.82
(2,742)	1:34:A:VAL:HG13	1:34:A:VAL:H	8	0.82
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD21	3	0.82
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	2	0.82
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	5	0.82
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB3	3	0.82
(2,873)	1:22:A:ILE:HD11	1:31:A:PRO:HD2	10	0.81
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	7	0.81
(2,745)	1:33:A:ILE:H	1:32:A:VAL:HG12	8	0.81
(2,732)	1:51:A:LEU:HD22	1:51:A:LEU:HB2	10	0.81
(2,679)	1:85:A:LEU:HD13	1:85:A:LEU:HA	9	0.81
(2,431)	1:120:A:SER:HB2	1:121:A:PRO:HD2	8	0.81
(2,345)	1:98:A:GLU:H	1:98:A:GLU:HG3	10	0.81
(1,211)	1:33:A:ILE:HD13	1:49:A:LYS:HD3	4	0.81
(1,108)	1:47:A:LYS:HE3	1:35:A:GLU:HB3	1	0.81
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD11	3	0.8
(2,742)	1:34:A:VAL:HG11	1:34:A:VAL:H	5	0.8
(2,742)	1:34:A:VAL:HG11	1:34:A:VAL:H	10	0.8
(2,739)	1:108:A:VAL:HG11	1:108:A:VAL:H	3	0.8
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	8	0.8
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB2	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:32:A:VAL:HG22	1:61:A:PHE:HE1	2	0.8
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	3	0.8
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	4	0.8
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD13	2	0.79
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD12	8	0.79
(2,742)	1:34:A:VAL:HG13	1:34:A:VAL:H	4	0.79
(2,742)	1:34:A:VAL:HG11	1:34:A:VAL:H	9	0.79
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD23	6	0.79
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG23	1	0.79
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG23	2	0.79
(1,228)	1:32:A:VAL:HG21	1:106:A:LEU:HD23	5	0.79
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	6	0.79
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	3	0.79
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	6	0.79
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	6	0.79
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG13	3	0.79
(2,860)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	2	0.78
(2,860)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	3	0.78
(2,742)	1:34:A:VAL:HG13	1:34:A:VAL:H	2	0.78
(2,742)	1:34:A:VAL:HG13	1:34:A:VAL:H	6	0.78
(2,742)	1:34:A:VAL:HG11	1:34:A:VAL:H	7	0.78
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	9	0.78
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	5	0.78
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	8	0.78
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	2	0.78
(2,1016)	1:34:A:VAL:HG12	1:45:A:ILE:HG23	10	0.77
(2,930)	1:3:A:LYS:HE3	1:3:A:LYS:HG3	1	0.77
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD13	1	0.77
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD13	4	0.77
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD11	7	0.77
(2,783)	1:109:A:THR:HG22	1:35:A:GLU:HB3	5	0.77
(2,742)	1:34:A:VAL:HG13	1:34:A:VAL:H	3	0.77
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG22	5	0.77
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG3	8	0.77
(1,234)	1:88:A:ALA:HB2	1:58:A:VAL:HB	6	0.77
(1,191)	1:65:A:ILE:HG22	1:45:A:ILE:HG23	7	0.77
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB1	5	0.77
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB3	7	0.77
(1,137)	1:45:A:ILE:HG13	1:69:A:ILE:HD11	10	0.77
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	1	0.77
(1,125)	1:65:A:ILE:HB	1:77:A:ILE:HG13	8	0.77
(1,125)	1:65:A:ILE:HB	1:45:A:ILE:HD11	10	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD11	1	0.77
(2,822)	1:76:A:ALA:HB2	1:67:A:LYS:HD3	5	0.76
(2,742)	1:34:A:VAL:HG11	1:34:A:VAL:H	1	0.76
(2,326)	1:28:A:ASP:H	1:27:A:PRO:HB3	10	0.76
(1,234)	1:88:A:ALA:HB2	1:58:A:VAL:HB	1	0.76
(1,181)	1:22:A:ILE:HG22	1:29:A:ARG:HG3	7	0.76
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB1	6	0.76
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB3	10	0.76
(1,168)	1:62:A:VAL:HG12	1:65:A:ILE:HD12	4	0.76
(1,137)	1:45:A:ILE:HG12	1:69:A:ILE:HD11	1	0.76
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	9	0.76
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD12	5	0.76
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD12	10	0.76
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	2	0.76
(2,955)	1:44:A:THR:HG22	1:70:A:LYS:HG3	6	0.75
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD11	5	0.75
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB3	10	0.75
(2,431)	1:120:A:SER:HB2	1:121:A:PRO:HD2	6	0.75
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	7	0.75
(1,234)	1:88:A:ALA:HB1	1:58:A:VAL:HB	5	0.75
(1,234)	1:88:A:ALA:HB3	1:58:A:VAL:HB	8	0.75
(1,234)	1:88:A:ALA:HB2	1:58:A:VAL:HB	9	0.75
(1,234)	1:88:A:ALA:HB1	1:58:A:VAL:HB	10	0.75
(1,200)	1:42:A:ILE:HG23	1:69:A:ILE:HD12	2	0.75
(1,190)	1:69:A:ILE:HG21	1:45:A:ILE:HG23	3	0.75
(1,182)	1:30:A:ILE:HG22	1:32:A:VAL:HB	10	0.75
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB1	8	0.75
(1,155)	1:44:A:THR:H	1:44:A:THR:HG22	5	0.75
(1,155)	1:44:A:THR:H	1:44:A:THR:HG23	9	0.75
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	6	0.75
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	8	0.75
(1,77)	1:94:A:SER:HB3	1:98:A:GLU:HB2	10	0.75
(1,69)	1:32:A:VAL:HG23	1:108:A:VAL:HG21	7	0.75
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	6	0.75
(2,1016)	1:34:A:VAL:HG12	1:45:A:ILE:HG23	7	0.74
(2,739)	1:108:A:VAL:HG12	1:108:A:VAL:H	7	0.74
(2,464)	1:12:A:LEU:HA	1:15:A:ARG:HB3	10	0.74
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG21	10	0.74
(1,234)	1:88:A:ALA:HB1	1:58:A:VAL:HB	3	0.74
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG11	8	0.74
(1,155)	1:44:A:THR:H	1:44:A:THR:HG23	2	0.74
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	4	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:65:A:ILE:HB	1:45:A:ILE:HD11	9	0.74
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	3	0.74
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD13	5	0.74
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD12	6	0.74
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	9	0.74
(2,1016)	1:34:A:VAL:HG12	1:45:A:ILE:HG23	1	0.73
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD13	8	0.73
(2,842)	1:30:A:ILE:HG21	1:96:A:TYR:HB2	5	0.73
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB2	1	0.73
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD13	8	0.73
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	6	0.73
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG12	4	0.73
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG21	6	0.73
(1,234)	1:88:A:ALA:HB3	1:58:A:VAL:HB	2	0.73
(1,228)	1:32:A:VAL:HG23	1:106:A:LEU:HD22	4	0.73
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG13	7	0.73
(1,168)	1:62:A:VAL:HG12	1:65:A:ILE:HD12	3	0.73
(1,168)	1:62:A:VAL:HG12	1:65:A:ILE:HD11	5	0.73
(1,155)	1:44:A:THR:H	1:44:A:THR:HG21	3	0.73
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD11	6	0.73
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA2	9	0.73
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	8	0.73
(2,873)	1:22:A:ILE:HD11	1:31:A:PRO:HD2	8	0.72
(2,842)	1:30:A:ILE:HG22	1:96:A:TYR:HB2	4	0.72
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG23	3	0.72
(2,739)	1:108:A:VAL:HG11	1:108:A:VAL:H	10	0.72
(2,704)	1:85:A:LEU:HD23	1:80:A:PHE:HE1	9	0.72
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	3	0.72
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	9	0.72
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	10	0.72
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG23	8	0.72
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG22	9	0.72
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD21	6	0.72
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD22	10	0.72
(1,200)	1:42:A:ILE:HG23	1:69:A:ILE:HD12	1	0.72
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB3	1	0.72
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD12	6	0.72
(1,158)	1:32:A:VAL:HG21	1:61:A:PHE:HE2	4	0.72
(1,155)	1:44:A:THR:H	1:44:A:THR:HG21	1	0.72
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	2	0.72
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD12	10	0.72
(1,105)	1:80:A:PHE:HB2	1:109:A:THR:HB	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	1	0.72
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE2	9	0.72
(2,875)	1:92:A:MET:HE3	1:61:A:PHE:HB3	4	0.71
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG13	2	0.71
(2,739)	1:108:A:VAL:HG13	1:108:A:VAL:H	8	0.71
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	5	0.71
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG21	8	0.71
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG23	9	0.71
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD12	9	0.71
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD11	10	0.71
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG12	4	0.71
(1,163)	1:57:A:THR:HG21	1:91:A:LEU:HB2	2	0.71
(1,155)	1:44:A:THR:H	1:44:A:THR:HG21	4	0.71
(1,137)	1:45:A:ILE:HG13	1:69:A:ILE:HD13	8	0.71
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	5	0.71
(2,842)	1:30:A:ILE:HG22	1:96:A:TYR:HB2	7	0.7
(2,753)	1:115:A:THR:HG22	1:116:A:PHE:HD2	6	0.7
(2,739)	1:108:A:VAL:HG13	1:108:A:VAL:H	1	0.7
(2,739)	1:108:A:VAL:HG13	1:108:A:VAL:H	5	0.7
(2,739)	1:108:A:VAL:HG11	1:108:A:VAL:H	9	0.7
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	2	0.7
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	8	0.7
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD13	1	0.7
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG22	3	0.7
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD23	4	0.7
(1,234)	1:88:A:ALA:HB1	1:58:A:VAL:HB	7	0.7
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG22	7	0.7
(1,192)	1:51:A:LEU:HD23	1:22:A:ILE:HG23	10	0.7
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB3	4	0.7
(1,137)	1:45:A:ILE:HG13	1:69:A:ILE:HD11	7	0.7
(1,125)	1:65:A:ILE:HB	1:45:A:ILE:HD11	5	0.7
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD12	8	0.7
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD13	8	0.7
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	7	0.7
(2,875)	1:92:A:MET:HE1	1:61:A:PHE:HB3	9	0.69
(2,823)	1:76:A:ALA:HB3	1:77:A:ILE:HG23	2	0.69
(2,739)	1:108:A:VAL:HG13	1:108:A:VAL:H	4	0.69
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	6	0.69
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	6	0.69
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD13	7	0.69
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG23	7	0.69
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD21	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD22	8	0.69
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG12	5	0.69
(1,226)	1:98:A:GLU:HB2	1:95:A:VAL:HG13	10	0.69
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD11	9	0.69
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	7	0.69
(1,129)	1:25:A:LYS:HB2	1:24:A:GLU:HB2	10	0.69
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD13	9	0.69
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	5	0.69
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	7	0.69
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB3	9	0.68
(2,739)	1:108:A:VAL:HG13	1:108:A:VAL:H	2	0.68
(2,675)	1:45:A:ILE:HG13	1:45:A:ILE:HG23	4	0.68
(2,447)	1:94:A:SER:HB3	1:91:A:LEU:HB3	2	0.68
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	1	0.68
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	8	0.68
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	1	0.68
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	9	0.68
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG23	4	0.68
(1,226)	1:95:A:VAL:HG11	1:100:A:LYS:HB3	3	0.68
(1,211)	1:33:A:ILE:HD12	1:49:A:LYS:HD3	2	0.68
(1,211)	1:33:A:ILE:HD11	1:49:A:LYS:HD2	5	0.68
(1,205)	1:65:A:ILE:HD12	1:62:A:VAL:HG21	1	0.68
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB1	9	0.68
(1,155)	1:44:A:THR:H	1:44:A:THR:HG21	10	0.68
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD13	9	0.68
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG13	4	0.68
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG12	8	0.68
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	9	0.68
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	2	0.68
(2,965)	1:32:A:VAL:HG23	1:32:A:VAL:HA	8	0.67
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	3	0.67
(2,875)	1:92:A:MET:HE2	1:61:A:PHE:HB3	6	0.67
(2,868)	1:92:A:MET:HE3	1:61:A:PHE:HE2	7	0.67
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG12	5	0.67
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG22	10	0.67
(1,234)	1:88:A:ALA:HB3	1:58:A:VAL:HB	4	0.67
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB3	7	0.67
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB3	3	0.67
(1,155)	1:44:A:THR:H	1:44:A:THR:HG22	8	0.67
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG11	7	0.67
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG11	9	0.67
(2,1012)	1:22:A:ILE:HG23	1:25:A:LYS:HD3	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG23	4	0.66
(2,875)	1:92:A:MET:HE3	1:61:A:PHE:HB3	2	0.66
(2,868)	1:92:A:MET:HE1	1:61:A:PHE:HE2	3	0.66
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG11	8	0.66
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB1	6	0.66
(2,711)	1:51:A:LEU:HD21	1:51:A:LEU:HA	1	0.66
(2,711)	1:51:A:LEU:HD21	1:51:A:LEU:HA	5	0.66
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	5	0.66
(2,464)	1:12:A:LEU:HA	1:15:A:ARG:HB3	6	0.66
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	4	0.66
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB2	10	0.66
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB1	8	0.66
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD22	7	0.66
(1,228)	1:32:A:VAL:HG21	1:106:A:LEU:HD22	2	0.66
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG22	9	0.66
(1,200)	1:42:A:ILE:HG22	1:69:A:ILE:HD12	3	0.66
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG22	9	0.66
(1,179)	1:22:A:ILE:HG23	1:31:A:PRO:HG3	10	0.66
(1,155)	1:44:A:THR:H	1:44:A:THR:HG21	7	0.66
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD12	2	0.66
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG11	7	0.66
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	6	0.66
(2,1012)	1:22:A:ILE:HG21	1:25:A:LYS:HD2	3	0.65
(2,1012)	1:22:A:ILE:HG22	1:25:A:LYS:HD2	7	0.65
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG23	1	0.65
(2,875)	1:92:A:MET:HE2	1:61:A:PHE:HB3	10	0.65
(2,846)	1:33:A:ILE:HG21	1:35:A:GLU:HG3	3	0.65
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG13	4	0.65
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG12	6	0.65
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG12	10	0.65
(2,803)	1:62:A:VAL:HG12	1:76:A:ALA:HB2	7	0.65
(2,739)	1:108:A:VAL:HG12	1:108:A:VAL:H	6	0.65
(2,711)	1:51:A:LEU:HD23	1:51:A:LEU:HA	2	0.65
(2,711)	1:51:A:LEU:HD23	1:51:A:LEU:HA	3	0.65
(2,711)	1:51:A:LEU:HD21	1:51:A:LEU:HA	4	0.65
(2,711)	1:51:A:LEU:HD21	1:51:A:LEU:HA	6	0.65
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB1	3	0.65
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB2	5	0.65
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB2	7	0.65
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB1	9	0.65
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB1	10	0.65
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	4	0.65
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD13	8	0.65
(2,78)	1:78:A:PHE:H	1:79:A:ILE:HG22	5	0.65
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG21	5	0.65
(1,181)	1:22:A:ILE:HG22	1:29:A:ARG:HG3	9	0.65
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB1	2	0.65
(1,137)	1:45:A:ILE:HG12	1:69:A:ILE:HD11	3	0.65
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	3	0.65
(2,1035)	1:32:A:VAL:HG23	1:92:A:MET:HE1	3	0.64
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD13	8	0.64
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	7	0.64
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG23	6	0.64
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG22	7	0.64
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG22	9	0.64
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD13	6	0.64
(2,842)	1:30:A:ILE:HG22	1:96:A:TYR:HB2	6	0.64
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG11	7	0.64
(2,711)	1:51:A:LEU:HD22	1:51:A:LEU:HA	7	0.64
(2,711)	1:51:A:LEU:HD23	1:51:A:LEU:HA	9	0.64
(2,609)	1:98:A:GLU:HG3	1:98:A:GLU:HA	10	0.64
(2,431)	1:120:A:SER:HB2	1:121:A:PRO:HD2	3	0.64
(2,395)	1:89:A:GLY:H	1:59:A:GLY:HA2	4	0.64
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD13	3	0.64
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	4	0.64
(1,168)	1:62:A:VAL:HG13	1:65:A:ILE:HD11	2	0.64
(1,62)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	10	0.64
(2,975)	1:58:A:VAL:HG11	1:92:A:MET:HG2	3	0.63
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG22	3	0.63
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG23	4	0.63
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG22	8	0.63
(2,875)	1:92:A:MET:HE2	1:61:A:PHE:HB3	5	0.63
(2,873)	1:22:A:ILE:HD11	1:31:A:PRO:HD2	7	0.63
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB1	1	0.63
(2,846)	1:33:A:ILE:HG23	1:35:A:GLU:HG3	10	0.63
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG11	3	0.63
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG13	9	0.63
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB3	5	0.63
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	3	0.63
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD21	5	0.63
(1,200)	1:42:A:ILE:HG22	1:69:A:ILE:HD13	10	0.63
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB1	2	0.63
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	7	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	8	0.63
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD11	7	0.63
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG11	10	0.63
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	4	0.63
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG11	10	0.63
(2,1032)	1:77:A:ILE:HG22	1:77:A:ILE:HD11	2	0.62
(2,965)	1:32:A:VAL:HG23	1:32:A:VAL:HA	7	0.62
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG23	2	0.62
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG23	5	0.62
(2,875)	1:92:A:MET:HE2	1:61:A:PHE:HB3	1	0.62
(2,843)	1:17:A:ALA:HB2	1:18:A:GLU:HB2	10	0.62
(2,813)	1:64:A:VAL:H	1:64:A:VAL:HG11	1	0.62
(2,766)	1:52:A:VAL:HG22	1:52:A:VAL:HA	1	0.62
(2,609)	1:98:A:GLU:HG3	1:98:A:GLU:HA	3	0.62
(2,609)	1:98:A:GLU:HG3	1:98:A:GLU:HA	4	0.62
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD13	2	0.62
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB2	4	0.62
(2,434)	1:72:A:SER:HB3	1:75:A:LYS:HG2	6	0.62
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG23	1	0.62
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG21	5	0.62
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB3	4	0.62
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB3	6	0.62
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	7	0.62
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG21	5	0.62
(1,104)	1:3:A:LYS:HE2	1:2:A:ALA:HA	6	0.62
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE3	2	0.62
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	1	0.62
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD11	5	0.61
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD13	10	0.61
(2,974)	1:115:A:THR:HG23	1:116:A:PHE:HB3	6	0.61
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	4	0.61
(2,842)	1:30:A:ILE:HG21	1:96:A:TYR:HB2	2	0.61
(2,823)	1:76:A:ALA:HB1	1:77:A:ILE:HG22	8	0.61
(2,805)	1:44:A:THR:HG22	1:45:A:ILE:HG21	5	0.61
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG12	2	0.61
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB2	3	0.61
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	6	0.61
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB1	2	0.61
(1,212)	1:33:A:ILE:HD11	1:49:A:LYS:HG3	3	0.61
(1,200)	1:42:A:ILE:HG22	1:69:A:ILE:HD12	7	0.61
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB3	4	0.61
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	1	0.61
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG11	5	0.61
(1,52)	1:97:A:GLU:H	1:95:A:VAL:HG13	5	0.61
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE3	5	0.61
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	5	0.61
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	10	0.61
(2,1012)	1:22:A:ILE:HG22	1:25:A:LYS:HD2	9	0.6
(2,893)	1:65:A:ILE:HG13	1:65:A:ILE:HG23	10	0.6
(2,875)	1:92:A:MET:HE1	1:61:A:PHE:HB3	8	0.6
(2,842)	1:30:A:ILE:HG21	1:96:A:TYR:HB2	1	0.6
(2,842)	1:30:A:ILE:HG21	1:96:A:TYR:HB2	3	0.6
(2,803)	1:62:A:VAL:HG13	1:76:A:ALA:HB1	4	0.6
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD11	3	0.6
(2,609)	1:98:A:GLU:HG3	1:98:A:GLU:HA	9	0.6
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB1	6	0.6
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG21	4	0.6
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	9	0.6
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD11	6	0.6
(2,3)	1:37:A:ALA:H	1:36:A:LYS:HB2	9	0.6
(1,248)	1:50:A:TYR:HE1	1:52:A:VAL:HB	2	0.6
(1,197)	1:45:A:ILE:HG22	1:69:A:ILE:HA	9	0.6
(1,178)	1:33:A:ILE:HG21	1:6:A:PHE:HB3	10	0.6
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB1	8	0.6
(1,137)	1:45:A:ILE:HG12	1:69:A:ILE:HD11	2	0.6
(1,137)	1:45:A:ILE:HG12	1:69:A:ILE:HD11	6	0.6
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG21	7	0.6
(1,95)	1:90:A:ALA:HA	1:58:A:VAL:HG23	3	0.6
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD12	7	0.59
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG21	3	0.59
(2,1012)	1:22:A:ILE:HG23	1:25:A:LYS:HD2	4	0.59
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD11	6	0.59
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB2	6	0.59
(2,846)	1:33:A:ILE:HG21	1:35:A:GLU:HG3	2	0.59
(2,823)	1:76:A:ALA:HB2	1:77:A:ILE:HG22	7	0.59
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG22	1	0.59
(2,738)	1:71:A:LEU:HD11	1:77:A:ILE:HG23	3	0.59
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG23	5	0.59
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG23	10	0.59
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG12	8	0.59
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB3	7	0.59
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	4	0.59
(2,147)	1:56:A:LEU:H	1:54:A:ALA:HB3	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD13	4	0.59
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD11	5	0.59
(1,200)	1:42:A:ILE:HG23	1:69:A:ILE:HD11	8	0.59
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB1	9	0.59
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG22	3	0.59
(1,110)	1:110:A:TYR:HB2	1:34:A:VAL:HG21	10	0.59
(2,1012)	1:22:A:ILE:HG21	1:25:A:LYS:HD2	1	0.58
(2,1005)	1:88:A:ALA:HB2	1:62:A:VAL:HG23	3	0.58
(2,967)	1:32:A:VAL:HG23	1:108:A:VAL:HG22	10	0.58
(2,868)	1:92:A:MET:HE3	1:61:A:PHE:HE2	8	0.58
(2,846)	1:33:A:ILE:HG21	1:35:A:GLU:HG3	9	0.58
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG22	6	0.58
(2,766)	1:52:A:VAL:HG21	1:52:A:VAL:HA	3	0.58
(2,766)	1:52:A:VAL:HG23	1:52:A:VAL:HA	8	0.58
(2,541)	1:70:A:LYS:HE3	1:43:A:PRO:HA	6	0.58
(2,483)	1:116:A:PHE:HA	1:116:A:PHE:HD2	4	0.58
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB3	9	0.58
(2,447)	1:94:A:SER:HB3	1:91:A:LEU:HB3	10	0.58
(2,414)	1:111:A:SER:HB3	1:37:A:ALA:HB1	2	0.58
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	5	0.58
(1,216)	1:5:A:SER:HA	1:8:A:GLN:HG2	10	0.58
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG21	5	0.58
(1,191)	1:65:A:ILE:HG23	1:45:A:ILE:HG21	3	0.58
(1,189)	1:79:A:ILE:HG23	1:108:A:VAL:HG12	10	0.58
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG22	6	0.58
(1,162)	1:32:A:VAL:HG23	1:106:A:LEU:HB3	9	0.58
(1,152)	1:109:A:THR:HG23	1:80:A:PHE:H	5	0.58
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG21	10	0.58
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG22	6	0.58
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	8	0.58
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD11	6	0.57
(2,1032)	1:77:A:ILE:HG22	1:77:A:ILE:HD11	9	0.57
(2,1016)	1:34:A:VAL:HG12	1:45:A:ILE:HG22	5	0.57
(2,805)	1:44:A:THR:HG23	1:45:A:ILE:HG21	9	0.57
(2,799)	1:108:A:VAL:HG12	1:92:A:MET:HE3	4	0.57
(2,799)	1:108:A:VAL:HG13	1:92:A:MET:HE1	10	0.57
(2,766)	1:52:A:VAL:HG21	1:52:A:VAL:HA	4	0.57
(2,766)	1:52:A:VAL:HG23	1:52:A:VAL:HA	5	0.57
(2,766)	1:52:A:VAL:HG22	1:52:A:VAL:HA	6	0.57
(2,766)	1:52:A:VAL:HG22	1:52:A:VAL:HA	9	0.57
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB3	1	0.57
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB2	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	9	0.57
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB1	1	0.57
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	1	0.57
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	4	0.57
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	2	0.57
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD11	1	0.57
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG21	4	0.57
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	5	0.57
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG21	8	0.57
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG23	9	0.57
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	8	0.57
(1,15)	1:11:A:ASP:H	1:10:A:HIS:HB3	10	0.57
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD11	3	0.56
(2,842)	1:30:A:ILE:HG22	1:96:A:TYR:HB2	9	0.56
(2,823)	1:76:A:ALA:HB1	1:77:A:ILE:HG22	6	0.56
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB3	2	0.56
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	2	0.56
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB3	8	0.56
(2,447)	1:94:A:SER:HB3	1:91:A:LEU:HB3	5	0.56
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	5	0.56
(2,79)	1:46:A:ASP:H	1:45:A:ILE:HD12	2	0.56
(1,228)	1:32:A:VAL:HG22	1:106:A:LEU:HD23	3	0.56
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	9	0.56
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG22	8	0.56
(1,191)	1:65:A:ILE:HG23	1:42:A:ILE:HD12	5	0.56
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG12	9	0.56
(1,186)	1:30:A:ILE:HG21	1:106:A:LEU:HB3	3	0.56
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	1	0.56
(1,18)	1:19:A:ALA:H	1:31:A:PRO:HG2	7	0.56
(1,17)	1:35:A:GLU:H	1:108:A:VAL:HB	1	0.56
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG12	4	0.56
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG13	5	0.56
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG11	7	0.56
(2,1032)	1:77:A:ILE:HG21	1:77:A:ILE:HD11	4	0.55
(2,994)	1:81:A:VAL:HG21	1:81:A:VAL:HG23	1	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG23	3	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	4	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	5	0.55
(2,994)	1:81:A:VAL:HG21	1:81:A:VAL:HG23	6	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	7	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	8	0.55
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	10	0.55
(2,965)	1:32:A:VAL:HG23	1:32:A:VAL:HA	10	0.55
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	5	0.55
(2,846)	1:33:A:ILE:HG23	1:35:A:GLU:HG3	7	0.55
(2,843)	1:17:A:ALA:HB1	1:18:A:GLU:HB2	5	0.55
(2,805)	1:44:A:THR:HG22	1:45:A:ILE:HG22	8	0.55
(2,803)	1:62:A:VAL:HG11	1:76:A:ALA:HB1	8	0.55
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB3	1	0.55
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	1	0.55
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE3	3	0.55
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE3	9	0.55
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	1	0.55
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	3	0.55
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	7	0.55
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	8	0.55
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	9	0.55
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD21	4	0.55
(2,447)	1:94:A:SER:HB3	1:91:A:LEU:HB3	6	0.55
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG3	2	0.55
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	5	0.55
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	8	0.55
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD23	2	0.55
(1,231)	1:57:A:THR:HG21	1:60:A:GLN:HB2	7	0.55
(1,226)	1:95:A:VAL:HG11	1:100:A:LYS:HB2	9	0.55
(1,208)	1:93:A:SER:H	1:30:A:ILE:HD12	7	0.55
(1,205)	1:65:A:ILE:HD12	1:62:A:VAL:HG22	4	0.55
(1,205)	1:65:A:ILE:HD12	1:62:A:VAL:HG22	6	0.55
(1,189)	1:79:A:ILE:HG23	1:108:A:VAL:HG12	3	0.55
(1,137)	1:45:A:ILE:HG13	1:69:A:ILE:HD11	5	0.55
(1,137)	1:45:A:ILE:HG13	1:69:A:ILE:HD13	9	0.55
(1,120)	1:113:A:GLU:H	1:113:A:GLU:HG3	1	0.55
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG22	8	0.55
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG21	3	0.55
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	4	0.55
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG13	8	0.55
(2,1032)	1:77:A:ILE:HG22	1:77:A:ILE:HD11	1	0.54
(2,994)	1:81:A:VAL:HG22	1:81:A:VAL:HG21	2	0.54
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG22	2	0.54
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	1	0.54
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	2	0.54
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD12	9	0.54
(2,912)	1:54:A:ALA:HA	1:30:A:ILE:HD13	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,873)	1:22:A:ILE:HD11	1:31:A:PRO:HD2	9	0.54
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB1	10	0.54
(2,842)	1:30:A:ILE:HG21	1:96:A:TYR:HB2	10	0.54
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG22	7	0.54
(2,780)	1:115:A:THR:HG21	1:116:A:PHE:HB3	9	0.54
(2,766)	1:52:A:VAL:HG22	1:52:A:VAL:HA	2	0.54
(2,754)	1:34:A:VAL:HG21	1:50:A:TYR:HE1	8	0.54
(2,699)	1:71:A:LEU:HD11	1:76:A:ALA:H	10	0.54
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD11	7	0.54
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	4	0.54
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	5	0.54
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	6	0.54
(2,489)	1:74:A:GLU:HA	1:74:A:GLU:HB3	10	0.54
(2,414)	1:111:A:SER:HB3	1:37:A:ALA:HB3	4	0.54
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD11	8	0.54
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	6	0.54
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	10	0.54
(1,197)	1:45:A:ILE:HG22	1:69:A:ILE:HA	10	0.54
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	5	0.54
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG23	9	0.54
(1,158)	1:32:A:VAL:HG21	1:61:A:PHE:HE1	9	0.54
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG22	6	0.54
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE3	3	0.54
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG12	4	0.54
(2,1012)	1:22:A:ILE:HG23	1:25:A:LYS:HD2	5	0.53
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD13	4	0.53
(2,843)	1:17:A:ALA:HB1	1:18:A:GLU:HB2	7	0.53
(2,823)	1:76:A:ALA:HB2	1:77:A:ILE:HG22	3	0.53
(2,818)	1:54:A:ALA:HB2	1:28:A:ASP:HB3	9	0.53
(2,805)	1:44:A:THR:HG23	1:45:A:ILE:HG21	2	0.53
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG23	3	0.53
(2,803)	1:62:A:VAL:HG13	1:76:A:ALA:HB2	3	0.53
(2,798)	1:109:A:THR:HG23	1:37:A:ALA:HB2	3	0.53
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	8	0.53
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE1	4	0.53
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG3	6	0.53
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB3	2	0.53
(2,3)	1:37:A:ALA:H	1:36:A:LYS:HB2	3	0.53
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	8	0.53
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	10	0.53
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	1	0.53
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:104:A:GLY:HA2	1:19:A:ALA:HB3	10	0.53
(1,170)	1:80:A:PHE:H	1:79:A:ILE:HG22	10	0.53
(1,163)	1:64:A:VAL:HG21	1:52:A:VAL:HB	3	0.53
(1,160)	1:12:A:LEU:HD12	1:103:A:ASP:HB3	4	0.53
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG22	1	0.53
(1,19)	1:95:A:VAL:H	1:90:A:ALA:HB1	3	0.53
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	2	0.53
(1,9)	1:108:A:VAL:H	1:107:A:TYR:HE2	8	0.53
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG11	9	0.53
(2,975)	1:58:A:VAL:HG13	1:92:A:MET:HG2	7	0.52
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG22	9	0.52
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG23	4	0.52
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG23	7	0.52
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	7	0.52
(2,324)	1:28:A:ASP:H	1:28:A:ASP:HB2	7	0.52
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	6	0.52
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	1	0.52
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	4	0.52
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	6	0.52
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	9	0.52
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	2	0.52
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	8	0.52
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB3	8	0.52
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB3	9	0.52
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	1	0.52
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	2	0.52
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG22	7	0.52
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG23	9	0.52
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD11	5	0.52
(1,248)	1:50:A:TYR:HE2	1:32:A:VAL:HB	8	0.52
(1,226)	1:95:A:VAL:HG12	1:100:A:LYS:HB3	6	0.52
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG21	2	0.52
(1,205)	1:65:A:ILE:HD12	1:62:A:VAL:HG22	3	0.52
(1,205)	1:65:A:ILE:HD11	1:62:A:VAL:HG23	9	0.52
(1,190)	1:69:A:ILE:HG21	1:45:A:ILE:HG22	4	0.52
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	2	0.52
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	4	0.52
(1,189)	1:79:A:ILE:HG23	1:108:A:VAL:HG13	6	0.52
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	7	0.52
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG21	2	0.52
(1,74)	1:72:A:SER:HB2	1:75:A:LYS:HG3	4	0.52
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG22	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG12	6	0.52
(2,1016)	1:34:A:VAL:HG12	1:45:A:ILE:HG23	9	0.51
(2,1012)	1:22:A:ILE:HG23	1:25:A:LYS:HD2	2	0.51
(2,848)	1:73:A:ALA:HB1	1:74:A:GLU:HB3	4	0.51
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG23	3	0.51
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG21	6	0.51
(2,753)	1:115:A:THR:HG23	1:116:A:PHE:HD2	7	0.51
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	9	0.51
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB1	6	0.51
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB2	8	0.51
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB1	9	0.51
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	5	0.51
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	8	0.51
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	10	0.51
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	1	0.51
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	3	0.51
(1,248)	1:50:A:TYR:HE1	1:52:A:VAL:HB	4	0.51
(1,248)	1:50:A:TYR:HE1	1:32:A:VAL:HB	6	0.51
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	2	0.51
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD13	8	0.51
(1,200)	1:42:A:ILE:HG21	1:69:A:ILE:HD12	4	0.51
(1,197)	1:45:A:ILE:HG21	1:69:A:ILE:HA	5	0.51
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG21	2	0.51
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	5	0.51
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG13	7	0.51
(1,186)	1:30:A:ILE:HG22	1:106:A:LEU:HB2	1	0.51
(1,181)	1:22:A:ILE:HG22	1:29:A:ARG:HG3	3	0.51
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD11	2	0.51
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG11	10	0.51
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	5	0.51
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE2	7	0.51
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	4	0.51
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG12	2	0.51
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG13	1	0.51
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG22	2	0.5
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG23	6	0.5
(2,1012)	1:22:A:ILE:HG21	1:25:A:LYS:HD2	8	0.5
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD11	4	0.5
(2,848)	1:73:A:ALA:HB2	1:74:A:GLU:HB3	10	0.5
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB3	5	0.5
(2,843)	1:17:A:ALA:HB3	1:18:A:GLU:HB2	2	0.5
(2,843)	1:17:A:ALA:HB2	1:18:A:GLU:HB2	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG21	1	0.5
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG22	4	0.5
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG22	8	0.5
(2,799)	1:108:A:VAL:HG12	1:92:A:MET:HE2	2	0.5
(2,783)	1:109:A:THR:HG23	1:35:A:GLU:HB3	10	0.5
(2,753)	1:115:A:THR:HG23	1:116:A:PHE:HD1	3	0.5
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	4	0.5
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD13	1	0.5
(2,324)	1:28:A:ASP:H	1:28:A:ASP:HB2	4	0.5
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	3	0.5
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	10	0.5
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG3	8	0.5
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD11	1	0.5
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD13	9	0.5
(2,114)	1:58:A:VAL:H	1:57:A:THR:HG21	3	0.5
(1,235)	1:88:A:ALA:HB2	1:88:A:ALA:HB1	9	0.5
(1,200)	1:42:A:ILE:HG22	1:69:A:ILE:HD12	5	0.5
(1,191)	1:65:A:ILE:HG21	1:45:A:ILE:HG22	2	0.5
(1,189)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	8	0.5
(1,177)	1:79:A:ILE:HG22	1:110:A:TYR:HB2	10	0.5
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG22	3	0.5
(1,152)	1:109:A:THR:HG23	1:80:A:PHE:H	6	0.5
(1,20)	1:109:A:THR:H	1:80:A:PHE:HB2	6	0.5
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	5	0.5
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG13	1	0.5
(1,5)	1:50:A:TYR:H	1:52:A:VAL:HG13	3	0.5
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG23	10	0.49
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD12	7	0.49
(2,884)	1:22:A:ILE:HD12	1:31:A:PRO:HB3	8	0.49
(2,852)	1:20:A:ALA:HB1	1:23:A:ARG:HG3	1	0.49
(2,846)	1:33:A:ILE:HG23	1:35:A:GLU:HG3	6	0.49
(2,843)	1:17:A:ALA:HB2	1:18:A:GLU:HB2	3	0.49
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG22	7	0.49
(2,818)	1:54:A:ALA:HB3	1:28:A:ASP:HB3	3	0.49
(2,799)	1:108:A:VAL:HG12	1:92:A:MET:HE3	8	0.49
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG21	10	0.49
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	2	0.49
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	3	0.49
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD11	7	0.49
(2,324)	1:28:A:ASP:H	1:28:A:ASP:HB2	2	0.49
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	2	0.49
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:25:A:LYS:H	1:25:A:LYS:HG2	7	0.49
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD11	10	0.49
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG22	2	0.49
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG23	10	0.49
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD12	6	0.49
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB2	7	0.49
(2,143)	1:75:A:LYS:H	1:75:A:LYS:HB3	4	0.49
(1,235)	1:73:A:ALA:HB2	1:73:A:ALA:HB1	1	0.49
(1,235)	1:73:A:ALA:HB2	1:73:A:ALA:HB3	2	0.49
(1,235)	1:88:A:ALA:HB1	1:88:A:ALA:HB3	3	0.49
(1,235)	1:88:A:ALA:HB1	1:88:A:ALA:HB3	4	0.49
(1,235)	1:88:A:ALA:HB1	1:88:A:ALA:HB3	5	0.49
(1,235)	1:88:A:ALA:HB2	1:88:A:ALA:HB3	6	0.49
(1,235)	1:88:A:ALA:HB1	1:88:A:ALA:HB3	7	0.49
(1,235)	1:88:A:ALA:HB1	1:88:A:ALA:HB3	8	0.49
(1,235)	1:88:A:ALA:HB1	1:88:A:ALA:HB3	10	0.49
(1,208)	1:93:A:SER:H	1:30:A:ILE:HD12	4	0.49
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG23	8	0.49
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG22	1	0.49
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG22	10	0.49
(1,173)	1:104:A:GLY:H	1:19:A:ALA:HB1	5	0.49
(1,163)	1:64:A:VAL:HG22	1:52:A:VAL:HB	7	0.49
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG2	10	0.49
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	10	0.49
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD12	3	0.49
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE3	1	0.49
(1,17)	1:35:A:GLU:H	1:108:A:VAL:HB	3	0.49
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG11	3	0.49
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG23	4	0.48
(2,884)	1:22:A:ILE:HD11	1:31:A:PRO:HB3	4	0.48
(2,843)	1:17:A:ALA:HB2	1:18:A:GLU:HB2	6	0.48
(2,843)	1:17:A:ALA:HB3	1:18:A:GLU:HB2	8	0.48
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG22	5	0.48
(2,820)	1:84:A:VAL:HB	1:81:A:VAL:HG22	10	0.48
(2,799)	1:108:A:VAL:HG12	1:92:A:MET:HE2	5	0.48
(2,777)	1:12:A:LEU:HD13	1:103:A:ASP:HB2	5	0.48
(2,766)	1:52:A:VAL:HG22	1:52:A:VAL:HA	7	0.48
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	3	0.48
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	9	0.48
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB2	4	0.48
(2,113)	1:92:A:MET:H	1:57:A:THR:HG23	9	0.48
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG21	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	7	0.48
(1,197)	1:45:A:ILE:HG22	1:69:A:ILE:HA	7	0.48
(1,190)	1:69:A:ILE:HG21	1:45:A:ILE:HG22	6	0.48
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG22	7	0.48
(1,163)	1:64:A:VAL:HG21	1:52:A:VAL:HB	1	0.48
(1,137)	1:45:A:ILE:HG12	1:69:A:ILE:HD11	4	0.48
(1,104)	1:47:A:LYS:HE3	1:5:A:SER:HB2	7	0.48
(1,104)	1:3:A:LYS:HE2	1:2:A:ALA:HA	9	0.48
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	9	0.48
(1,96)	1:87:A:PRO:HD2	1:95:A:VAL:HG21	9	0.48
(1,77)	1:94:A:SER:HB3	1:98:A:GLU:HB2	2	0.48
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	10	0.48
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG13	8	0.48
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	5	0.48
(1,54)	1:111:A:SER:H	1:78:A:PHE:HB2	6	0.48
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG23	1	0.48
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG21	5	0.48
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	6	0.48
(1,3)	1:76:A:ALA:H	1:77:A:ILE:H	9	0.48
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD13	3	0.47
(2,914)	1:92:A:MET:HE2	1:30:A:ILE:HD11	4	0.47
(2,914)	1:92:A:MET:HE1	1:30:A:ILE:HD13	6	0.47
(2,914)	1:92:A:MET:HE2	1:30:A:ILE:HD12	8	0.47
(2,898)	1:65:A:ILE:HD11	1:61:A:PHE:HD2	7	0.47
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD11	1	0.47
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB2	2	0.47
(2,843)	1:17:A:ALA:HB3	1:18:A:GLU:HB2	9	0.47
(2,822)	1:76:A:ALA:HB3	1:67:A:LYS:HD3	8	0.47
(2,818)	1:54:A:ALA:HB3	1:28:A:ASP:HB3	5	0.47
(2,803)	1:62:A:VAL:HG13	1:76:A:ALA:HB2	5	0.47
(2,799)	1:108:A:VAL:HG11	1:92:A:MET:HE2	6	0.47
(2,776)	1:12:A:LEU:HD11	1:16:A:ARG:HD3	1	0.47
(2,776)	1:12:A:LEU:HD11	1:16:A:ARG:HD3	5	0.47
(2,766)	1:52:A:VAL:HG21	1:52:A:VAL:HA	10	0.47
(2,753)	1:115:A:THR:HG21	1:116:A:PHE:HD1	9	0.47
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG21	8	0.47
(2,671)	1:70:A:LYS:HD3	1:70:A:LYS:HG3	6	0.47
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE2	7	0.47
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	4	0.47
(2,324)	1:28:A:ASP:H	1:28:A:ASP:HB2	6	0.47
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	5	0.47
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG21	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD12	10	0.47
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	1	0.47
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	5	0.47
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG21	5	0.47
(1,219)	1:3:A:LYS:HD2	1:3:A:LYS:HG3	10	0.47
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD12	3	0.47
(1,191)	1:65:A:ILE:HG21	1:45:A:ILE:HG23	1	0.47
(1,152)	1:109:A:THR:HG22	1:80:A:PHE:H	9	0.47
(1,148)	1:51:A:LEU:HD21	1:105:A:PHE:HE2	10	0.47
(1,107)	1:47:A:LYS:HE3	1:35:A:GLU:HG2	5	0.47
(1,69)	1:32:A:VAL:HG23	1:108:A:VAL:HG22	4	0.47
(1,69)	1:32:A:VAL:HG23	1:108:A:VAL:HG22	10	0.47
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	8	0.47
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	9	0.47
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	6	0.47
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	7	0.47
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG13	10	0.47
(2,1012)	1:22:A:ILE:HG22	1:25:A:LYS:HD2	10	0.46
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG22	2	0.46
(2,914)	1:92:A:MET:HE1	1:30:A:ILE:HD11	5	0.46
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD12	2	0.46
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD12	9	0.46
(2,884)	1:22:A:ILE:HD13	1:31:A:PRO:HB3	6	0.46
(2,884)	1:22:A:ILE:HD12	1:31:A:PRO:HB3	9	0.46
(2,868)	1:92:A:MET:HE2	1:61:A:PHE:HE2	2	0.46
(2,852)	1:20:A:ALA:HB2	1:23:A:ARG:HG3	4	0.46
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB1	6	0.46
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB2	9	0.46
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG21	3	0.46
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG21	9	0.46
(2,799)	1:108:A:VAL:HG13	1:92:A:MET:HE1	9	0.46
(2,786)	1:12:A:LEU:HD11	1:16:A:ARG:HB2	8	0.46
(2,776)	1:12:A:LEU:HD11	1:16:A:ARG:HD3	10	0.46
(2,541)	1:70:A:LYS:HE2	1:43:A:PRO:HA	9	0.46
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	4	0.46
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	5	0.46
(2,483)	1:116:A:PHE:HA	1:116:A:PHE:HD2	6	0.46
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD13	8	0.46
(2,414)	1:111:A:SER:HB3	1:37:A:ALA:HB3	10	0.46
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	10	0.46
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD12	5	0.46
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG22	1	0.46
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG21	2	0.46
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG22	3	0.46
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG23	9	0.46
(1,219)	1:3:A:LYS:HD2	1:3:A:LYS:HG3	6	0.46
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	2	0.46
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	7	0.46
(1,40)	1:70:A:LYS:H	1:71:A:LEU:HB2	6	0.46
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG21	4	0.46
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG11	8	0.46
(2,1016)	1:34:A:VAL:HG11	1:45:A:ILE:HG23	4	0.45
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD13	5	0.45
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD12	10	0.45
(2,869)	1:92:A:MET:HE3	1:58:A:VAL:HA	7	0.45
(2,848)	1:73:A:ALA:HB3	1:74:A:GLU:HB3	5	0.45
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB1	4	0.45
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB3	7	0.45
(2,818)	1:54:A:ALA:HB2	1:28:A:ASP:HB3	10	0.45
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG22	9	0.45
(2,776)	1:12:A:LEU:HD11	1:16:A:ARG:HD3	8	0.45
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	10	0.45
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	5	0.45
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	9	0.45
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	2	0.45
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	10	0.45
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB3	5	0.45
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG22	1	0.45
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG23	3	0.45
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	2	0.45
(2,173)	1:64:A:VAL:H	1:63:A:TYR:HB2	7	0.45
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD11	7	0.45
(1,228)	1:32:A:VAL:HG23	1:106:A:LEU:HD22	9	0.45
(1,224)	1:51:A:LEU:HD11	1:22:A:ILE:HG21	6	0.45
(1,186)	1:30:A:ILE:HG21	1:106:A:LEU:HB3	2	0.45
(1,181)	1:22:A:ILE:HG22	1:29:A:ARG:HG3	1	0.45
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG22	3	0.45
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	7	0.45
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB3	10	0.45
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD13	8	0.45
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG13	5	0.45
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG12	6	0.45
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG23	7	0.44
(2,1005)	1:88:A:ALA:HB1	1:62:A:VAL:HG22	2	0.44
(2,932)	1:113:A:GLU:HG2	1:75:A:LYS:HG3	1	0.44
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD13	3	0.44
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD13	6	0.44
(2,884)	1:22:A:ILE:HD11	1:31:A:PRO:HB3	1	0.44
(2,858)	1:20:A:ALA:HB2	1:19:A:ALA:HB1	10	0.44
(2,843)	1:17:A:ALA:HB3	1:18:A:GLU:HB2	1	0.44
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG21	2	0.44
(2,699)	1:71:A:LEU:HD13	1:76:A:ALA:H	4	0.44
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	1	0.44
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	3	0.44
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	5	0.44
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	1	0.44
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	2	0.44
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	3	0.44
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	6	0.44
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	7	0.44
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	8	0.44
(2,521)	1:43:A:PRO:HD2	1:43:A:PRO:HA	10	0.44
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE3	10	0.44
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	6	0.44
(2,436)	1:65:A:ILE:HA	1:45:A:ILE:HD12	9	0.44
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD13	6	0.44
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD13	5	0.44
(2,113)	1:92:A:MET:H	1:57:A:THR:HG22	7	0.44
(2,18)	1:85:A:LEU:H	1:85:A:LEU:HD21	9	0.44
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	5	0.44
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG23	10	0.44
(1,179)	1:22:A:ILE:HG22	1:31:A:PRO:HG3	3	0.44
(1,179)	1:22:A:ILE:HG21	1:31:A:PRO:HG3	6	0.44
(1,179)	1:22:A:ILE:HG23	1:31:A:PRO:HG3	7	0.44
(1,179)	1:22:A:ILE:HG23	1:31:A:PRO:HG3	9	0.44
(1,155)	1:44:A:THR:H	1:44:A:THR:HG21	6	0.44
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG22	6	0.44
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG13	1	0.44
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG13	4	0.44
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD12	6	0.44
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD11	9	0.44
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG11	5	0.44
(2,975)	1:58:A:VAL:HG13	1:92:A:MET:HG2	4	0.43
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG23	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD12	2	0.43
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD12	10	0.43
(2,940)	1:85:A:LEU:HD21	1:85:A:LEU:HD23	1	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD23	2	0.43
(2,940)	1:85:A:LEU:HD21	1:85:A:LEU:HD23	3	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD21	4	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD21	5	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD21	6	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD23	7	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD21	8	0.43
(2,940)	1:85:A:LEU:HD22	1:85:A:LEU:HD23	9	0.43
(2,940)	1:85:A:LEU:HD21	1:85:A:LEU:HD23	10	0.43
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD21	9	0.43
(2,914)	1:92:A:MET:HE1	1:30:A:ILE:HD11	1	0.43
(2,890)	1:77:A:ILE:HG23	1:42:A:ILE:HD12	10	0.43
(2,884)	1:22:A:ILE:HD13	1:31:A:PRO:HB3	3	0.43
(2,884)	1:22:A:ILE:HD13	1:31:A:PRO:HB3	5	0.43
(2,873)	1:22:A:ILE:HD12	1:31:A:PRO:HD2	3	0.43
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB2	5	0.43
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB1	3	0.43
(2,779)	1:109:A:THR:HG23	1:80:A:PHE:HB2	6	0.43
(2,776)	1:12:A:LEU:HD11	1:16:A:ARG:HD3	2	0.43
(2,716)	1:62:A:VAL:HG23	1:59:A:GLY:HA3	5	0.43
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG23	5	0.43
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG21	8	0.43
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE1	2	0.43
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD12	6	0.43
(2,470)	1:18:A:GLU:HA	1:17:A:ALA:HB1	10	0.43
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG23	2	0.43
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG22	7	0.43
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG21	10	0.43
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD12	9	0.43
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	10	0.43
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	2	0.43
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	4	0.43
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	5	0.43
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	6	0.43
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	7	0.43
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	8	0.43
(2,102)	1:11:A:ASP:H	1:12:A:LEU:HA	4	0.43
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG2	2	0.43
(2,3)	1:37:A:ALA:H	1:36:A:LYS:HB2	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:32:A:VAL:HG11	1:32:A:VAL:HG13	1	0.43
(1,227)	1:32:A:VAL:HG11	1:32:A:VAL:HG13	2	0.43
(1,227)	1:32:A:VAL:HG12	1:32:A:VAL:HG11	3	0.43
(1,227)	1:32:A:VAL:HG11	1:32:A:VAL:HG13	4	0.43
(1,227)	1:34:A:VAL:HG11	1:34:A:VAL:HG13	5	0.43
(1,227)	1:32:A:VAL:HG12	1:32:A:VAL:HG11	6	0.43
(1,227)	1:32:A:VAL:HG11	1:32:A:VAL:HG13	7	0.43
(1,227)	1:32:A:VAL:HG11	1:32:A:VAL:HG13	8	0.43
(1,227)	1:32:A:VAL:HG12	1:32:A:VAL:HG13	9	0.43
(1,227)	1:32:A:VAL:HG11	1:32:A:VAL:HG13	10	0.43
(1,224)	1:51:A:LEU:HD11	1:22:A:ILE:HG23	7	0.43
(1,211)	1:33:A:ILE:HD11	1:49:A:LYS:HD2	7	0.43
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	5	0.43
(1,190)	1:69:A:ILE:HG23	1:45:A:ILE:HG22	8	0.43
(1,181)	1:22:A:ILE:HG21	1:29:A:ARG:HG3	4	0.43
(1,177)	1:79:A:ILE:HG22	1:110:A:TYR:HB2	6	0.43
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG21	9	0.43
(1,152)	1:109:A:THR:HG22	1:80:A:PHE:H	2	0.43
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	2	0.43
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD12	4	0.43
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	1	0.43
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	3	0.43
(2,1037)	1:92:A:MET:HE2	1:92:A:MET:HE3	7	0.42
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG21	1	0.42
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD11	1	0.42
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD13	5	0.42
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD12	6	0.42
(2,971)	1:57:A:THR:HG22	1:91:A:LEU:HD11	7	0.42
(2,971)	1:57:A:THR:HG21	1:91:A:LEU:HD13	8	0.42
(2,939)	1:85:A:LEU:HD23	1:85:A:LEU:HD11	4	0.42
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD12	8	0.42
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD13	9	0.42
(2,884)	1:22:A:ILE:HD12	1:31:A:PRO:HB3	2	0.42
(2,873)	1:22:A:ILE:HD11	1:31:A:PRO:HD2	2	0.42
(2,868)	1:92:A:MET:HE1	1:61:A:PHE:HE2	10	0.42
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB2	1	0.42
(2,847)	1:21:A:ARG:HB3	1:17:A:ALA:HB2	8	0.42
(2,823)	1:76:A:ALA:HB3	1:77:A:ILE:HG23	9	0.42
(2,776)	1:12:A:LEU:HD11	1:16:A:ARG:HD3	7	0.42
(2,764)	1:109:A:THR:HG23	1:37:A:ALA:HA	9	0.42
(2,716)	1:62:A:VAL:HG21	1:59:A:GLY:HA3	10	0.42
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD11	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG21	3	0.42
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG21	6	0.42
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	8	0.42
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG22	3	0.42
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE3	1	0.42
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE3	5	0.42
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE3	6	0.42
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD13	5	0.42
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD11	9	0.42
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD13	10	0.42
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG21	8	0.42
(2,440)	1:6:A:PHE:HA	1:6:A:PHE:HD2	6	0.42
(2,434)	1:72:A:SER:HB3	1:75:A:LYS:HG2	10	0.42
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB1	3	0.42
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	6	0.42
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	8	0.42
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD11	8	0.42
(2,189)	1:71:A:LEU:H	1:71:A:LEU:HG	9	0.42
(2,150)	1:47:A:LYS:H	1:45:A:ILE:HG21	6	0.42
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	2	0.42
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	1	0.42
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	10	0.42
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	7	0.42
(1,231)	1:57:A:THR:HG22	1:60:A:GLN:HB2	9	0.42
(1,219)	1:3:A:LYS:HD3	1:3:A:LYS:HG2	4	0.42
(1,208)	1:93:A:SER:H	1:30:A:ILE:HD13	10	0.42
(1,163)	1:64:A:VAL:HG21	1:52:A:VAL:HB	9	0.42
(1,154)	1:109:A:THR:HG23	1:37:A:ALA:H	7	0.42
(1,139)	1:85:A:LEU:HD11	1:78:A:PHE:HE2	8	0.42
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	4	0.42
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG22	9	0.42
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG11	3	0.42
(1,62)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	6	0.42
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	9	0.42
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD11	7	0.42
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD13	5	0.42
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	4	0.42
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	7	0.42
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	5	0.42
(2,1037)	1:92:A:MET:HE1	1:92:A:MET:HE3	1	0.41
(2,1037)	1:92:A:MET:HE2	1:92:A:MET:HE3	2	0.41
(2,1037)	1:92:A:MET:HE1	1:92:A:MET:HE3	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1037)	1:92:A:MET:HE1	1:92:A:MET:HE3	4	0.41
(2,1037)	1:92:A:MET:HE1	1:92:A:MET:HE3	5	0.41
(2,1037)	1:92:A:MET:HE2	1:92:A:MET:HE3	6	0.41
(2,1037)	1:92:A:MET:HE1	1:92:A:MET:HE3	8	0.41
(2,1037)	1:92:A:MET:HE2	1:92:A:MET:HE3	9	0.41
(2,1037)	1:92:A:MET:HE2	1:92:A:MET:HE1	10	0.41
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG23	1	0.41
(2,914)	1:92:A:MET:HE1	1:30:A:ILE:HD11	2	0.41
(2,894)	1:22:A:ILE:H	1:22:A:ILE:HD12	8	0.41
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB1	9	0.41
(2,798)	1:109:A:THR:HG21	1:37:A:ALA:HB2	7	0.41
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG23	1	0.41
(2,716)	1:62:A:VAL:HG21	1:59:A:GLY:HA3	7	0.41
(2,716)	1:62:A:VAL:HG21	1:59:A:GLY:HA3	8	0.41
(2,716)	1:62:A:VAL:HG22	1:59:A:GLY:HA3	9	0.41
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG23	1	0.41
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG21	4	0.41
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG22	9	0.41
(2,699)	1:71:A:LEU:HD12	1:76:A:ALA:H	2	0.41
(2,699)	1:71:A:LEU:HD12	1:76:A:ALA:H	5	0.41
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD13	2	0.41
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	7	0.41
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	4	0.41
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	3	0.41
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	4	0.41
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD12	2	0.41
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	9	0.41
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG2	9	0.41
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	4	0.41
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD12	2	0.41
(1,200)	1:42:A:ILE:HG21	1:69:A:ILE:HD12	6	0.41
(1,152)	1:109:A:THR:HG21	1:80:A:PHE:H	10	0.41
(1,146)	1:71:A:LEU:HG	1:77:A:ILE:HG21	9	0.41
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	2	0.41
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	5	0.41
(1,89)	1:56:A:LEU:HA	1:91:A:LEU:HD13	3	0.41
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD13	8	0.41
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD13	10	0.41
(1,17)	1:35:A:GLU:H	1:108:A:VAL:HB	4	0.41
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	9	0.41
(1,17)	1:35:A:GLU:H	1:34:A:VAL:HB	10	0.41
(2,1005)	1:88:A:ALA:HB3	1:62:A:VAL:HG21	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,971)	1:57:A:THR:HG23	1:91:A:LEU:HD13	9	0.4
(2,914)	1:92:A:MET:HE3	1:30:A:ILE:HD12	10	0.4
(2,898)	1:65:A:ILE:HD12	1:61:A:PHE:HD2	10	0.4
(2,892)	1:69:A:ILE:HG23	1:69:A:ILE:HD11	2	0.4
(2,873)	1:22:A:ILE:HD12	1:31:A:PRO:HD2	5	0.4
(2,868)	1:92:A:MET:HE3	1:61:A:PHE:HE1	4	0.4
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD13	1	0.4
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD13	10	0.4
(2,858)	1:20:A:ALA:HB2	1:19:A:ALA:HB2	2	0.4
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB1	3	0.4
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB3	4	0.4
(2,822)	1:76:A:ALA:HB1	1:67:A:LYS:HD3	1	0.4
(2,799)	1:108:A:VAL:HG12	1:92:A:MET:HE2	1	0.4
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG22	4	0.4
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG22	10	0.4
(2,786)	1:12:A:LEU:HD13	1:16:A:ARG:HB2	5	0.4
(2,786)	1:12:A:LEU:HD13	1:16:A:ARG:HB2	7	0.4
(2,716)	1:62:A:VAL:HG21	1:59:A:GLY:HA3	6	0.4
(2,705)	1:62:A:VAL:HG21	1:61:A:PHE:HD1	1	0.4
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD2	3	0.4
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD1	6	0.4
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG21	7	0.4
(2,699)	1:71:A:LEU:HD12	1:76:A:ALA:H	1	0.4
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD11	1	0.4
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD12	5	0.4
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	4	0.4
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	4	0.4
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	5	0.4
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	8	0.4
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG13	1	0.4
(2,541)	1:70:A:LYS:HE3	1:43:A:PRO:HA	10	0.4
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	2	0.4
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB2	2	0.4
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	7	0.4
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	8	0.4
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	2	0.4
(1,211)	1:33:A:ILE:HD13	1:49:A:LYS:HD2	10	0.4
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD12	1	0.4
(1,208)	1:96:A:TYR:H	1:30:A:ILE:HD11	6	0.4
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG22	1	0.4
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG23	3	0.4
(1,181)	1:22:A:ILE:HG21	1:29:A:ARG:HG3	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:22:A:ILE:HG21	1:31:A:PRO:HG3	2	0.4
(1,167)	1:65:A:ILE:HD13	1:34:A:VAL:HG22	10	0.4
(1,162)	1:32:A:VAL:HG23	1:106:A:LEU:HB3	4	0.4
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	6	0.4
(1,77)	1:94:A:SER:HB2	1:98:A:GLU:HB2	1	0.4
(1,77)	1:94:A:SER:HB2	1:98:A:GLU:HB2	9	0.4
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG13	2	0.4
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG11	9	0.4
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	3	0.4
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD12	6	0.4
(1,20)	1:109:A:THR:H	1:3:A:LYS:HE2	8	0.4
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	9	0.4
(1,15)	1:11:A:ASP:H	1:10:A:HIS:HB3	6	0.4
(2,1054)	1:107:A:TYR:HD1	1:107:A:TYR:HB2	10	0.39
(2,1033)	1:69:A:ILE:HG23	1:65:A:ILE:HG22	8	0.39
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB1	7	0.39
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB2	9	0.39
(2,939)	1:85:A:LEU:HD21	1:85:A:LEU:HD12	1	0.39
(2,932)	1:113:A:GLU:HG2	1:75:A:LYS:HG3	8	0.39
(2,914)	1:92:A:MET:HE3	1:30:A:ILE:HD11	9	0.39
(2,884)	1:22:A:ILE:HD12	1:31:A:PRO:HB3	10	0.39
(2,873)	1:22:A:ILE:HD13	1:31:A:PRO:HD2	4	0.39
(2,873)	1:22:A:ILE:HD12	1:31:A:PRO:HD2	6	0.39
(2,872)	1:92:A:MET:HE3	1:61:A:PHE:HB2	4	0.39
(2,872)	1:92:A:MET:HE1	1:61:A:PHE:HB2	10	0.39
(2,868)	1:92:A:MET:HE1	1:61:A:PHE:HE2	9	0.39
(2,858)	1:20:A:ALA:HB1	1:19:A:ALA:HB1	4	0.39
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB1	7	0.39
(2,858)	1:20:A:ALA:HB2	1:19:A:ALA:HB2	9	0.39
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB1	10	0.39
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG21	1	0.39
(2,818)	1:54:A:ALA:HB1	1:28:A:ASP:HB3	1	0.39
(2,777)	1:12:A:LEU:HD11	1:103:A:ASP:HB2	8	0.39
(2,776)	1:12:A:LEU:HD12	1:16:A:ARG:HD3	4	0.39
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG11	1	0.39
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG11	2	0.39
(2,716)	1:62:A:VAL:HG23	1:59:A:GLY:HA3	1	0.39
(2,716)	1:62:A:VAL:HG23	1:59:A:GLY:HA3	2	0.39
(2,716)	1:62:A:VAL:HG21	1:59:A:GLY:HA3	3	0.39
(2,716)	1:62:A:VAL:HG21	1:59:A:GLY:HA3	4	0.39
(2,705)	1:62:A:VAL:HG21	1:61:A:PHE:HD2	5	0.39
(2,703)	1:63:A:TYR:H	1:62:A:VAL:HG23	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	2	0.39
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	1	0.39
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	3	0.39
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	6	0.39
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	7	0.39
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	9	0.39
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	10	0.39
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD22	4	0.39
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG21	10	0.39
(2,497)	1:92:A:MET:HA	1:92:A:MET:HE2	8	0.39
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	1	0.39
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	5	0.39
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	10	0.39
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD13	6	0.39
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	9	0.39
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD13	8	0.39
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	8	0.39
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG2	1	0.39
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	6	0.39
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	3	0.39
(1,208)	1:93:A:SER:H	1:30:A:ILE:HD12	5	0.39
(1,206)	1:65:A:ILE:HD13	1:34:A:VAL:HG21	1	0.39
(1,206)	1:65:A:ILE:HD13	1:34:A:VAL:HG22	3	0.39
(1,197)	1:45:A:ILE:HG22	1:69:A:ILE:HA	1	0.39
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG21	10	0.39
(1,191)	1:65:A:ILE:HG22	1:42:A:ILE:HD12	4	0.39
(1,181)	1:22:A:ILE:HG21	1:29:A:ARG:HG3	5	0.39
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG22	5	0.39
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG22	1	0.39
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	7	0.39
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	5	0.39
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	3	0.39
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD12	1	0.39
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	7	0.39
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	8	0.39
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB3	10	0.39
(1,41)	1:80:A:PHE:H	1:81:A:VAL:HG23	2	0.39
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD11	8	0.39
(1,4)	1:76:A:ALA:H	1:75:A:LYS:HB3	5	0.39
(2,1062)	1:50:A:TYR:HE2	1:64:A:VAL:HG12	3	0.38
(2,1001)	1:58:A:VAL:HG13	1:88:A:ALA:HB3	2	0.38
(2,1001)	1:58:A:VAL:HG12	1:88:A:ALA:HB1	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB3	4	0.38
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG13	9	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG23	1	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG23	2	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG23	3	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG22	4	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG22	5	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG23	6	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG22	7	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG22	8	0.38
(2,972)	1:109:A:THR:HG21	1:109:A:THR:HG23	9	0.38
(2,972)	1:109:A:THR:HG22	1:109:A:THR:HG23	10	0.38
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD11	6	0.38
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD12	10	0.38
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD23	4	0.38
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD22	10	0.38
(2,914)	1:92:A:MET:HE3	1:30:A:ILE:HD11	3	0.38
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD11	7	0.38
(2,872)	1:92:A:MET:HE3	1:61:A:PHE:HB2	8	0.38
(2,870)	1:42:A:ILE:HD12	1:67:A:LYS:HA	8	0.38
(2,846)	1:33:A:ILE:HG23	1:35:A:GLU:HG3	4	0.38
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB3	2	0.38
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB1	5	0.38
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB1	7	0.38
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB3	8	0.38
(2,823)	1:76:A:ALA:HB2	1:77:A:ILE:HG23	1	0.38
(2,798)	1:109:A:THR:HG23	1:37:A:ALA:HB2	6	0.38
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG22	2	0.38
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG22	5	0.38
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG22	7	0.38
(2,770)	1:115:A:THR:HG22	1:115:A:THR:HA	6	0.38
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG11	8	0.38
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG12	6	0.38
(2,707)	1:58:A:VAL:HG23	1:57:A:THR:HA	1	0.38
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD12	9	0.38
(2,665)	1:39:A:LYS:HA	1:39:A:LYS:HD2	9	0.38
(2,636)	1:8:A:GLN:HG2	1:9:A:GLU:HB2	3	0.38
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG23	7	0.38
(2,476)	1:60:A:GLN:HA	1:56:A:LEU:HD11	3	0.38
(2,413)	1:111:A:SER:HB2	1:37:A:ALA:HB1	7	0.38
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB2	3	0.38
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG21	6	0.38
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	1	0.38
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	6	0.38
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG23	9	0.38
(1,211)	1:33:A:ILE:HD13	1:49:A:LYS:HD3	9	0.38
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	4	0.38
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG23	2	0.38
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG22	7	0.38
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	7	0.38
(1,165)	1:52:A:VAL:HG22	1:52:A:VAL:HG12	5	0.38
(1,160)	1:12:A:LEU:HD11	1:103:A:ASP:HB3	2	0.38
(1,148)	1:51:A:LEU:HD22	1:105:A:PHE:HE2	4	0.38
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG21	10	0.38
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA3	7	0.38
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	3	0.38
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	7	0.38
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	6	0.38
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	1	0.38
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	2	0.38
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	8	0.38
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	10	0.38
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG21	2	0.37
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB1	10	0.37
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB2	1	0.37
(2,975)	1:58:A:VAL:HG13	1:92:A:MET:HG2	9	0.37
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	4	0.37
(2,864)	1:69:A:ILE:H	1:69:A:ILE:HD13	9	0.37
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB2	1	0.37
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB2	6	0.37
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG23	8	0.37
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB1	10	0.37
(2,798)	1:109:A:THR:HG23	1:37:A:ALA:HB3	8	0.37
(2,786)	1:12:A:LEU:HD13	1:16:A:ARG:HB2	10	0.37
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG13	3	0.37
(2,730)	1:71:A:LEU:HD11	1:67:A:LYS:HB2	10	0.37
(2,724)	1:51:A:LEU:HD21	1:29:A:ARG:HB2	8	0.37
(2,699)	1:71:A:LEU:HD12	1:76:A:ALA:H	6	0.37
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	9	0.37
(2,541)	1:70:A:LYS:HE3	1:43:A:PRO:HA	7	0.37
(2,328)	1:8:A:GLN:H	1:8:A:GLN:HB2	4	0.37
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD23	4	0.37
(2,267)	1:113:A:GLU:H	1:113:A:GLU:HG3	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	1	0.37
(1,219)	1:3:A:LYS:HD2	1:3:A:LYS:HG3	5	0.37
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG21	8	0.37
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	1	0.37
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	8	0.37
(1,148)	1:51:A:LEU:HD22	1:105:A:PHE:HE2	1	0.37
(1,133)	1:99:A:LYS:HB3	1:95:A:VAL:HG12	5	0.37
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	10	0.37
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	2	0.37
(1,67)	1:81:A:VAL:HB	1:108:A:VAL:HG12	7	0.37
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB3	5	0.37
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD12	3	0.37
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD12	4	0.37
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD11	9	0.37
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	7	0.37
(2,1054)	1:107:A:TYR:HD1	1:107:A:TYR:HB2	6	0.36
(2,1035)	1:32:A:VAL:HG23	1:92:A:MET:HE1	9	0.36
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG21	5	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB3	1	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB3	2	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB1	3	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB1	4	0.36
(2,1002)	1:17:A:ALA:HB1	1:17:A:ALA:HB3	5	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB1	6	0.36
(2,1002)	1:17:A:ALA:HB1	1:17:A:ALA:HB3	7	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB3	8	0.36
(2,1002)	1:17:A:ALA:HB2	1:17:A:ALA:HB3	9	0.36
(2,1001)	1:58:A:VAL:HG12	1:88:A:ALA:HB2	6	0.36
(2,1001)	1:58:A:VAL:HG12	1:88:A:ALA:HB1	10	0.36
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG12	4	0.36
(2,975)	1:58:A:VAL:HG13	1:92:A:MET:HG2	1	0.36
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	3	0.36
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD12	6	0.36
(2,888)	1:92:A:MET:HE2	1:108:A:VAL:HG21	3	0.36
(2,884)	1:22:A:ILE:HD12	1:31:A:PRO:HB3	7	0.36
(2,872)	1:92:A:MET:HE2	1:61:A:PHE:HB2	2	0.36
(2,870)	1:42:A:ILE:HD12	1:67:A:LYS:HA	6	0.36
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD12	9	0.36
(2,848)	1:73:A:ALA:HB2	1:74:A:GLU:HB3	6	0.36
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB1	3	0.36
(2,827)	1:88:A:ALA:H	1:88:A:ALA:HB2	9	0.36
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG23	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG23	6	0.36
(2,797)	1:91:A:LEU:HB3	1:95:A:VAL:HG23	8	0.36
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG13	4	0.36
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG13	5	0.36
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG11	6	0.36
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD13	9	0.36
(2,718)	1:3:A:LYS:HE3	1:3:A:LYS:HG2	2	0.36
(2,706)	1:85:A:LEU:HD21	1:78:A:PHE:HD2	3	0.36
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	9	0.36
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD23	2	0.36
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD22	5	0.36
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG22	3	0.36
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG21	7	0.36
(2,150)	1:47:A:LYS:H	1:45:A:ILE:HG23	5	0.36
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB2	1	0.36
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	4	0.36
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	3	0.36
(1,209)	1:30:A:ILE:HD13	1:106:A:LEU:HB2	6	0.36
(1,165)	1:32:A:VAL:HG21	1:32:A:VAL:HG11	1	0.36
(1,163)	1:64:A:VAL:HG21	1:52:A:VAL:HB	6	0.36
(1,146)	1:71:A:LEU:HG	1:77:A:ILE:HG23	3	0.36
(1,133)	1:99:A:LYS:HB3	1:95:A:VAL:HG13	10	0.36
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	7	0.36
(1,62)	1:79:A:ILE:HG21	1:65:A:ILE:HD12	3	0.36
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	9	0.36
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD11	5	0.36
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD12	10	0.36
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD11	7	0.36
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	2	0.36
(1,9)	1:108:A:VAL:H	1:107:A:TYR:HD1	3	0.36
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG11	1	0.35
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG11	2	0.35
(2,981)	1:108:A:VAL:HG11	1:108:A:VAL:HG13	3	0.35
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG11	4	0.35
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG11	5	0.35
(2,981)	1:108:A:VAL:HG11	1:108:A:VAL:HG13	6	0.35
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG11	8	0.35
(2,981)	1:108:A:VAL:HG11	1:108:A:VAL:HG13	9	0.35
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG13	10	0.35
(2,975)	1:58:A:VAL:HG13	1:92:A:MET:HG2	8	0.35
(2,962)	1:34:A:VAL:HG11	1:45:A:ILE:HG12	4	0.35
(2,939)	1:85:A:LEU:HD23	1:85:A:LEU:HD13	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,938)	1:71:A:LEU:HD12	1:115:A:THR:HG21	7	0.35
(2,938)	1:71:A:LEU:HD13	1:115:A:THR:HG23	10	0.35
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD22	8	0.35
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD11	8	0.35
(2,873)	1:22:A:ILE:HD13	1:31:A:PRO:HD2	1	0.35
(2,840)	1:42:A:ILE:HG21	1:40:A:SER:HB2	9	0.35
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG22	5	0.35
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG12	7	0.35
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	5	0.35
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	8	0.35
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	1	0.35
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	9	0.35
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	9	0.35
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD12	7	0.35
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD22	8	0.35
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG21	4	0.35
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG22	6	0.35
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG21	6	0.35
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB2	3	0.35
(2,102)	1:11:A:ASP:H	1:12:A:LEU:HA	2	0.35
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	1	0.35
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	6	0.35
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG3	10	0.35
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG23	2	0.35
(1,211)	1:33:A:ILE:HD11	1:49:A:LYS:HD2	3	0.35
(1,193)	1:52:A:VAL:HG22	1:30:A:ILE:HG23	10	0.35
(1,181)	1:22:A:ILE:HG21	1:29:A:ARG:HG3	2	0.35
(1,157)	1:34:A:VAL:HG22	1:61:A:PHE:HE1	10	0.35
(1,148)	1:51:A:LEU:HD22	1:105:A:PHE:HE2	6	0.35
(1,148)	1:51:A:LEU:HD23	1:105:A:PHE:HE2	7	0.35
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG21	9	0.35
(1,136)	1:29:A:ARG:HG3	1:22:A:ILE:HD13	5	0.35
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	1	0.35
(1,77)	1:94:A:SER:HB2	1:98:A:GLU:HB2	3	0.35
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	2	0.35
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	3	0.35
(1,62)	1:79:A:ILE:HG22	1:65:A:ILE:HD11	2	0.35
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB3	3	0.35
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD12	1	0.35
(1,37)	1:65:A:ILE:H	1:65:A:ILE:HD11	2	0.35
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG22	2	0.35
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG23	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	10	0.35
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	1	0.35
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG12	6	0.35
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB3	1	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB1	2	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB3	3	0.34
(2,1003)	1:20:A:ALA:HB1	1:20:A:ALA:HB3	4	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB3	5	0.34
(2,1003)	1:20:A:ALA:HB1	1:20:A:ALA:HB3	6	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB1	7	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB3	8	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB1	9	0.34
(2,1003)	1:20:A:ALA:HB2	1:20:A:ALA:HB1	10	0.34
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB3	8	0.34
(2,988)	1:76:A:ALA:HB1	1:76:A:ALA:HB3	1	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB1	2	0.34
(2,988)	1:76:A:ALA:HB1	1:76:A:ALA:HB3	3	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB3	4	0.34
(2,988)	1:76:A:ALA:HB1	1:76:A:ALA:HB3	5	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB3	6	0.34
(2,988)	1:76:A:ALA:HB1	1:76:A:ALA:HB3	7	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB3	8	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB1	9	0.34
(2,988)	1:76:A:ALA:HB2	1:76:A:ALA:HB1	10	0.34
(2,981)	1:108:A:VAL:HG12	1:108:A:VAL:HG11	7	0.34
(2,975)	1:58:A:VAL:HG12	1:92:A:MET:HG2	2	0.34
(2,975)	1:58:A:VAL:HG13	1:92:A:MET:HG2	5	0.34
(2,975)	1:58:A:VAL:HG11	1:92:A:MET:HG2	6	0.34
(2,975)	1:58:A:VAL:HG11	1:92:A:MET:HG2	10	0.34
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	7	0.34
(2,939)	1:85:A:LEU:HD22	1:85:A:LEU:HD13	5	0.34
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD23	7	0.34
(2,914)	1:92:A:MET:HE2	1:30:A:ILE:HD11	7	0.34
(2,870)	1:42:A:ILE:HD12	1:67:A:LYS:HA	10	0.34
(2,868)	1:92:A:MET:HE2	1:61:A:PHE:HE2	5	0.34
(2,858)	1:20:A:ALA:HB3	1:19:A:ALA:HB2	8	0.34
(2,770)	1:115:A:THR:HG21	1:115:A:THR:HA	8	0.34
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG11	9	0.34
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG11	4	0.34
(2,738)	1:71:A:LEU:HD12	1:77:A:ILE:HG23	6	0.34
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG23	2	0.34
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,711)	1:51:A:LEU:HD23	1:51:A:LEU:HA	8	0.34
(2,707)	1:58:A:VAL:HG21	1:57:A:THR:HA	3	0.34
(2,699)	1:71:A:LEU:HD11	1:76:A:ALA:H	3	0.34
(2,699)	1:71:A:LEU:HD11	1:76:A:ALA:H	8	0.34
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB2	10	0.34
(2,382)	1:55:A:ASP:H	1:55:A:ASP:HB3	9	0.34
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD12	2	0.34
(2,294)	1:23:A:ARG:H	1:23:A:ARG:HG3	7	0.34
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG22	2	0.34
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG21	3	0.34
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	2	0.34
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	1	0.34
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	2	0.34
(2,109)	1:92:A:MET:H	1:91:A:LEU:HB3	3	0.34
(2,80)	1:51:A:LEU:H	1:51:A:LEU:HD11	8	0.34
(1,248)	1:50:A:TYR:HE2	1:32:A:VAL:HB	5	0.34
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	5	0.34
(1,233)	1:84:A:VAL:HG21	1:86:A:PRO:HD3	10	0.34
(1,208)	1:93:A:SER:H	1:30:A:ILE:HD12	9	0.34
(1,188)	1:54:A:ALA:HB1	1:30:A:ILE:HG13	10	0.34
(1,186)	1:30:A:ILE:HG21	1:106:A:LEU:HB3	5	0.34
(1,179)	1:22:A:ILE:HG22	1:31:A:PRO:HG3	1	0.34
(1,165)	1:52:A:VAL:HG21	1:52:A:VAL:HG11	6	0.34
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG22	8	0.34
(1,148)	1:51:A:LEU:HD21	1:105:A:PHE:HE2	3	0.34
(1,136)	1:29:A:ARG:HG3	1:22:A:ILE:HD13	6	0.34
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	1	0.34
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	4	0.34
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	4	0.34
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	5	0.34
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	9	0.34
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HD2	7	0.34
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	2	0.34
(1,22)	1:18:A:GLU:H	1:21:A:ARG:HB3	5	0.34
(1,1)	1:82:A:ASP:H	1:81:A:VAL:HG11	2	0.34
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG13	1	0.33
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG13	1	0.33
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG11	2	0.33
(2,984)	1:58:A:VAL:HG11	1:58:A:VAL:HG13	3	0.33
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG13	4	0.33
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG13	5	0.33
(2,984)	1:58:A:VAL:HG11	1:58:A:VAL:HG13	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG13	7	0.33
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG13	8	0.33
(2,984)	1:58:A:VAL:HG12	1:58:A:VAL:HG13	9	0.33
(2,984)	1:58:A:VAL:HG11	1:58:A:VAL:HG13	10	0.33
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	1	0.33
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	2	0.33
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	5	0.33
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	6	0.33
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	8	0.33
(2,969)	1:57:A:THR:HG22	1:89:A:GLY:HA2	10	0.33
(2,938)	1:71:A:LEU:HD13	1:115:A:THR:HG21	3	0.33
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	6	0.33
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD12	3	0.33
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD12	4	0.33
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD11	9	0.33
(2,888)	1:92:A:MET:HE1	1:108:A:VAL:HG23	7	0.33
(2,882)	1:45:A:ILE:HG21	1:47:A:LYS:HB3	10	0.33
(2,869)	1:92:A:MET:HE1	1:58:A:VAL:HA	3	0.33
(2,868)	1:92:A:MET:HE2	1:61:A:PHE:HE1	6	0.33
(2,848)	1:73:A:ALA:HB3	1:74:A:GLU:HB3	1	0.33
(2,848)	1:73:A:ALA:HB1	1:74:A:GLU:HB3	8	0.33
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB3	1	0.33
(2,821)	1:76:A:ALA:HB1	1:67:A:LYS:HB3	6	0.33
(2,738)	1:71:A:LEU:HD12	1:77:A:ILE:HG21	1	0.33
(2,738)	1:71:A:LEU:HD12	1:77:A:ILE:HG23	5	0.33
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD11	3	0.33
(2,707)	1:58:A:VAL:HG22	1:57:A:THR:HA	9	0.33
(2,705)	1:62:A:VAL:HG23	1:61:A:PHE:HD2	9	0.33
(2,699)	1:71:A:LEU:HD13	1:76:A:ALA:H	7	0.33
(2,666)	1:70:A:LYS:HD2	1:70:A:LYS:HA	6	0.33
(2,555)	1:70:A:LYS:HE2	1:42:A:ILE:HG12	10	0.33
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG23	5	0.33
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	7	0.33
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB1	1	0.33
(2,382)	1:55:A:ASP:H	1:55:A:ASP:HB3	3	0.33
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG13	1	0.33
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD11	3	0.33
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD22	1	0.33
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD21	10	0.33
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	2	0.33
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	10	0.33
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	3	0.33
(1,248)	1:50:A:TYR:HE1	1:32:A:VAL:HB	3	0.33
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	3	0.33
(1,223)	1:71:A:LEU:HD13	1:42:A:ILE:HD13	5	0.33
(1,206)	1:65:A:ILE:HD13	1:34:A:VAL:HG21	6	0.33
(1,200)	1:42:A:ILE:HG23	1:69:A:ILE:HD11	9	0.33
(1,188)	1:54:A:ALA:HB3	1:30:A:ILE:HG13	6	0.33
(1,165)	1:32:A:VAL:HG23	1:32:A:VAL:HG13	3	0.33
(1,165)	1:52:A:VAL:HG23	1:52:A:VAL:HG11	4	0.33
(1,160)	1:12:A:LEU:HD13	1:15:A:ARG:HB2	7	0.33
(1,154)	1:109:A:THR:HG21	1:37:A:ALA:H	2	0.33
(1,148)	1:51:A:LEU:HD21	1:105:A:PHE:HE2	2	0.33
(1,146)	1:71:A:LEU:HG	1:77:A:ILE:HG23	10	0.33
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG22	6	0.33
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	5	0.33
(1,63)	1:79:A:ILE:HD11	1:62:A:VAL:HG21	3	0.33
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG21	7	0.33
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	3	0.33
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG22	9	0.32
(2,1001)	1:58:A:VAL:HG11	1:88:A:ALA:HB1	5	0.32
(2,899)	1:65:A:ILE:HD12	1:61:A:PHE:HE2	7	0.32
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD11	5	0.32
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD12	10	0.32
(2,889)	1:45:A:ILE:HG23	1:45:A:ILE:HD12	4	0.32
(2,868)	1:92:A:MET:HE2	1:61:A:PHE:HE1	1	0.32
(2,848)	1:73:A:ALA:HB1	1:74:A:GLU:HB3	2	0.32
(2,848)	1:73:A:ALA:HB3	1:74:A:GLU:HB3	7	0.32
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB1	4	0.32
(2,821)	1:76:A:ALA:HB1	1:67:A:LYS:HB3	8	0.32
(2,759)	1:108:A:VAL:HG21	1:108:A:VAL:HA	6	0.32
(2,753)	1:115:A:THR:HG22	1:116:A:PHE:HD2	4	0.32
(2,738)	1:71:A:LEU:HD11	1:77:A:ILE:HG23	10	0.32
(2,730)	1:71:A:LEU:HD13	1:67:A:LYS:HB2	4	0.32
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	10	0.32
(2,707)	1:58:A:VAL:HG21	1:57:A:THR:HA	2	0.32
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	4	0.32
(2,701)	1:85:A:LEU:HD21	1:79:A:ILE:H	9	0.32
(2,555)	1:70:A:LYS:HE2	1:42:A:ILE:HG12	7	0.32
(2,548)	1:39:A:LYS:HE3	1:39:A:LYS:HB2	9	0.32
(2,431)	1:120:A:SER:HB2	1:121:A:PRO:HD2	1	0.32
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB1	4	0.32
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB1	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB2	7	0.32
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB2	9	0.32
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD12	1	0.32
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	3	0.32
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	4	0.32
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG22	9	0.32
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	10	0.32
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	9	0.32
(1,236)	1:37:A:ALA:HB2	1:37:A:ALA:HB3	1	0.32
(1,236)	1:54:A:ALA:HB1	1:54:A:ALA:HB3	2	0.32
(1,236)	1:54:A:ALA:HB2	1:54:A:ALA:HB3	7	0.32
(1,236)	1:54:A:ALA:HB1	1:54:A:ALA:HB3	8	0.32
(1,236)	1:37:A:ALA:HB1	1:37:A:ALA:HB3	9	0.32
(1,236)	1:54:A:ALA:HB1	1:54:A:ALA:HB3	10	0.32
(1,224)	1:51:A:LEU:HD13	1:22:A:ILE:HG22	8	0.32
(1,219)	1:3:A:LYS:HD3	1:3:A:LYS:HG2	8	0.32
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	2	0.32
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	3	0.32
(1,209)	1:30:A:ILE:HD11	1:106:A:LEU:HB2	10	0.32
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	10	0.32
(1,180)	1:33:A:ILE:HG22	1:49:A:LYS:HB3	5	0.32
(1,169)	1:54:A:ALA:HB1	1:30:A:ILE:HD13	8	0.32
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	4	0.32
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	2	0.32
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	9	0.32
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD11	6	0.32
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	1	0.32
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB3	4	0.32
(2,1060)	1:107:A:TYR:HE1	1:3:A:LYS:HE2	2	0.31
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	10	0.31
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG22	8	0.31
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG23	9	0.31
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG13	2	0.31
(2,978)	1:81:A:VAL:HG11	1:3:A:LYS:HG2	2	0.31
(2,962)	1:34:A:VAL:HG11	1:45:A:ILE:HG12	2	0.31
(2,947)	1:71:A:LEU:HD12	1:71:A:LEU:HD13	3	0.31
(2,947)	1:71:A:LEU:HD12	1:71:A:LEU:HD11	4	0.31
(2,947)	1:71:A:LEU:HD12	1:71:A:LEU:HD11	7	0.31
(2,947)	1:71:A:LEU:HD12	1:71:A:LEU:HD13	10	0.31
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	2	0.31
(2,939)	1:85:A:LEU:HD21	1:85:A:LEU:HD11	2	0.31
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD21	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,901)	1:79:A:ILE:HD13	1:79:A:ILE:HB	9	0.31
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD12	1	0.31
(2,895)	1:65:A:ILE:H	1:65:A:ILE:HD11	2	0.31
(2,872)	1:92:A:MET:HE1	1:61:A:PHE:HB2	9	0.31
(2,848)	1:73:A:ALA:HB2	1:74:A:GLU:HB3	3	0.31
(2,848)	1:73:A:ALA:HB1	1:74:A:GLU:HB3	9	0.31
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB2	3	0.31
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB2	5	0.31
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB3	6	0.31
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB1	8	0.31
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB2	4	0.31
(2,779)	1:109:A:THR:HG23	1:80:A:PHE:HB2	5	0.31
(2,759)	1:108:A:VAL:HG21	1:108:A:VAL:HA	5	0.31
(2,753)	1:115:A:THR:HG22	1:116:A:PHE:HD2	10	0.31
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD12	5	0.31
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	4	0.31
(2,710)	1:58:A:VAL:HG23	1:57:A:THR:HB	3	0.31
(2,707)	1:58:A:VAL:HG22	1:57:A:THR:HA	6	0.31
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD2	7	0.31
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG11	3	0.31
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG21	6	0.31
(2,398)	1:89:A:GLY:H	1:87:A:PRO:HB3	3	0.31
(2,367)	1:40:A:SER:H	1:37:A:ALA:HB1	3	0.31
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD12	10	0.31
(2,315)	1:13:A:GLU:H	1:12:A:LEU:HD23	7	0.31
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG22	1	0.31
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG22	5	0.31
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG23	8	0.31
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	5	0.31
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG23	9	0.31
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	7	0.31
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD2	8	0.31
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD13	7	0.31
(2,187)	1:71:A:LEU:H	1:115:A:THR:HG21	3	0.31
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	5	0.31
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	8	0.31
(1,250)	1:107:A:TYR:HE2	1:6:A:PHE:HB2	7	0.31
(1,236)	1:54:A:ALA:HB1	1:54:A:ALA:HB3	3	0.31
(1,236)	1:54:A:ALA:HB2	1:54:A:ALA:HB3	4	0.31
(1,236)	1:54:A:ALA:HB2	1:54:A:ALA:HB1	5	0.31
(1,236)	1:54:A:ALA:HB2	1:54:A:ALA:HB3	6	0.31
(1,219)	1:3:A:LYS:HD3	1:3:A:LYS:HG2	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:54:A:ALA:HB1	1:30:A:ILE:HG13	2	0.31
(1,179)	1:22:A:ILE:HG21	1:31:A:PRO:HG3	4	0.31
(1,157)	1:34:A:VAL:HG21	1:61:A:PHE:HE2	7	0.31
(1,151)	1:51:A:LEU:HD22	1:22:A:ILE:HD11	1	0.31
(1,149)	1:51:A:LEU:HD11	1:105:A:PHE:HE2	8	0.31
(1,148)	1:51:A:LEU:HD22	1:105:A:PHE:HE2	5	0.31
(1,148)	1:51:A:LEU:HD23	1:105:A:PHE:HE2	8	0.31
(1,148)	1:51:A:LEU:HD21	1:105:A:PHE:HE2	9	0.31
(1,146)	1:71:A:LEU:HG	1:77:A:ILE:HG21	2	0.31
(1,142)	1:51:A:LEU:HG	1:22:A:ILE:HD12	10	0.31
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG21	4	0.31
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	3	0.31
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	8	0.31
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	8	0.31
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD11	1	0.31
(2,1029)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	3	0.3
(2,1015)	1:79:A:ILE:HG21	1:62:A:VAL:HG22	6	0.3
(2,1015)	1:79:A:ILE:HG21	1:62:A:VAL:HG22	10	0.3
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG12	3	0.3
(2,969)	1:57:A:THR:HG23	1:89:A:GLY:HA2	7	0.3
(2,947)	1:71:A:LEU:HD11	1:71:A:LEU:HD13	1	0.3
(2,947)	1:71:A:LEU:HD11	1:71:A:LEU:HD13	2	0.3
(2,947)	1:71:A:LEU:HD11	1:71:A:LEU:HD13	5	0.3
(2,947)	1:71:A:LEU:HD11	1:71:A:LEU:HD13	6	0.3
(2,947)	1:71:A:LEU:HD11	1:71:A:LEU:HD13	8	0.3
(2,947)	1:71:A:LEU:HD12	1:71:A:LEU:HD13	9	0.3
(2,938)	1:71:A:LEU:HD13	1:115:A:THR:HG21	8	0.3
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD21	1	0.3
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD12	9	0.3
(2,872)	1:92:A:MET:HE2	1:61:A:PHE:HB2	6	0.3
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG23	6	0.3
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB1	2	0.3
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB3	9	0.3
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB2	10	0.3
(2,818)	1:54:A:ALA:HB2	1:28:A:ASP:HB3	8	0.3
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB1	2	0.3
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB3	5	0.3
(2,784)	1:57:A:THR:HG21	1:60:A:GLN:HB2	7	0.3
(2,779)	1:109:A:THR:HG22	1:80:A:PHE:HB2	9	0.3
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG23	9	0.3
(2,718)	1:3:A:LYS:HE2	1:3:A:LYS:HG2	9	0.3
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,644)	1:113:A:GLU:H	1:113:A:GLU:HB2	1	0.3
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG12	3	0.3
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG13	3	0.3
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD13	10	0.3
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB3	5	0.3
(2,278)	1:80:A:PHE:H	1:79:A:ILE:HG22	10	0.3
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	5	0.3
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	6	0.3
(2,227)	1:30:A:ILE:H	1:30:A:ILE:HD12	6	0.3
(2,148)	1:18:A:GLU:H	1:19:A:ALA:HB3	6	0.3
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	6	0.3
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	2	0.3
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	4	0.3
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD13	3	0.3
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD12	10	0.3
(1,231)	1:57:A:THR:HG23	1:60:A:GLN:HB2	4	0.3
(1,197)	1:45:A:ILE:HG23	1:69:A:ILE:HA	3	0.3
(1,177)	1:79:A:ILE:HG23	1:110:A:TYR:HB2	5	0.3
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	9	0.3
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG21	6	0.3
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	5	0.3
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	1	0.3
(1,6)	1:54:A:ALA:H	1:55:A:ASP:HA	9	0.3
(2,1060)	1:107:A:TYR:HE1	1:3:A:LYS:HE2	3	0.29
(2,1046)	1:79:A:ILE:HD12	1:108:A:VAL:HG12	3	0.29
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	8	0.29
(2,1005)	1:88:A:ALA:HB3	1:62:A:VAL:HG22	1	0.29
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG23	4	0.29
(2,969)	1:57:A:THR:HG21	1:89:A:GLY:HA2	9	0.29
(2,959)	1:108:A:VAL:HG21	1:107:A:TYR:HA	2	0.29
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	5	0.29
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD22	5	0.29
(2,926)	1:79:A:ILE:HG12	1:85:A:LEU:HD22	6	0.29
(2,908)	1:77:A:ILE:HD12	1:79:A:ILE:HD11	8	0.29
(2,872)	1:92:A:MET:HE2	1:61:A:PHE:HB2	5	0.29
(2,870)	1:42:A:ILE:HD13	1:67:A:LYS:HA	7	0.29
(2,824)	1:59:A:GLY:H	1:88:A:ALA:HB2	7	0.29
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB3	3	0.29
(2,799)	1:108:A:VAL:HG13	1:92:A:MET:HE2	3	0.29
(2,779)	1:109:A:THR:HG22	1:80:A:PHE:HB2	1	0.29
(2,759)	1:108:A:VAL:HG23	1:108:A:VAL:HA	10	0.29
(2,738)	1:71:A:LEU:HD13	1:77:A:ILE:HG23	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,738)	1:71:A:LEU:HD11	1:77:A:ILE:HG23	8	0.29
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD1	4	0.29
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD2	10	0.29
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	3	0.29
(2,623)	1:8:A:GLN:H	1:8:A:GLN:HG2	3	0.29
(2,622)	1:75:A:LYS:HB2	1:76:A:ALA:H	7	0.29
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG12	4	0.29
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD21	7	0.29
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG21	4	0.29
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG12	5	0.29
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	6	0.29
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	8	0.29
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD2	7	0.29
(2,204)	1:103:A:ASP:H	1:101:A:ASP:HB2	10	0.29
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	6	0.29
(2,69)	1:61:A:PHE:H	1:60:A:GLN:HG2	7	0.29
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD13	8	0.29
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG22	7	0.29
(1,226)	1:95:A:VAL:HG11	1:100:A:LYS:HB2	2	0.29
(1,212)	1:33:A:ILE:HD13	1:49:A:LYS:HG2	4	0.29
(1,206)	1:65:A:ILE:HD12	1:34:A:VAL:HG21	2	0.29
(1,188)	1:54:A:ALA:HB1	1:30:A:ILE:HG13	7	0.29
(1,184)	1:69:A:ILE:HG23	1:45:A:ILE:HG13	5	0.29
(1,179)	1:22:A:ILE:HG21	1:31:A:PRO:HG3	5	0.29
(1,166)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	7	0.29
(1,166)	1:34:A:VAL:HG13	1:65:A:ILE:HD13	10	0.29
(1,165)	1:32:A:VAL:HG22	1:32:A:VAL:HG12	2	0.29
(1,162)	1:32:A:VAL:HG21	1:106:A:LEU:HB3	5	0.29
(1,159)	1:108:A:VAL:HG21	1:34:A:VAL:HA	7	0.29
(1,150)	1:71:A:LEU:HD12	1:42:A:ILE:HG13	10	0.29
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG22	8	0.29
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	1	0.29
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	2	0.29
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	4	0.29
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	7	0.29
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	9	0.29
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	4	0.29
(1,4)	1:76:A:ALA:H	1:75:A:LYS:HB3	10	0.29
(2,1046)	1:79:A:ILE:HD12	1:108:A:VAL:HG11	8	0.28
(2,1029)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	5	0.28
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	6	0.28
(2,1015)	1:79:A:ILE:HG21	1:62:A:VAL:HG22	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	8	0.28
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD11	3	0.28
(2,872)	1:92:A:MET:HE2	1:61:A:PHE:HB2	1	0.28
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG23	10	0.28
(2,786)	1:12:A:LEU:HD12	1:16:A:ARG:HB2	4	0.28
(2,784)	1:57:A:THR:HG23	1:60:A:GLN:HB2	8	0.28
(2,780)	1:115:A:THR:HG23	1:116:A:PHE:HB3	6	0.28
(2,759)	1:108:A:VAL:HG21	1:108:A:VAL:HA	8	0.28
(2,759)	1:108:A:VAL:HG21	1:108:A:VAL:HA	9	0.28
(2,751)	1:64:A:VAL:HG21	1:61:A:PHE:HD1	8	0.28
(2,750)	1:63:A:TYR:H	1:62:A:VAL:HG11	10	0.28
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG11	5	0.28
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG11	7	0.28
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG11	8	0.28
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD12	6	0.28
(2,730)	1:71:A:LEU:HD12	1:67:A:LYS:HB2	1	0.28
(2,730)	1:71:A:LEU:HD12	1:67:A:LYS:HB2	5	0.28
(2,730)	1:71:A:LEU:HD13	1:67:A:LYS:HB2	7	0.28
(2,707)	1:58:A:VAL:HG22	1:57:A:THR:HA	4	0.28
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	7	0.28
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	3	0.28
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	6	0.28
(2,554)	1:39:A:LYS:HE3	1:39:A:LYS:HD3	3	0.28
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG12	7	0.28
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD22	1	0.28
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD23	2	0.28
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD21	8	0.28
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG12	9	0.28
(2,454)	1:45:A:ILE:HA	1:45:A:ILE:HG21	9	0.28
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	7	0.28
(2,385)	1:55:A:ASP:H	1:54:A:ALA:HB2	8	0.28
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG13	2	0.28
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG12	6	0.28
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG11	9	0.28
(2,317)	1:79:A:ILE:H	1:79:A:ILE:HD12	4	0.28
(2,276)	1:70:A:LYS:H	1:44:A:THR:HG22	6	0.28
(2,273)	1:20:A:ALA:H	1:21:A:ARG:HG2	9	0.28
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	5	0.28
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	7	0.28
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	1	0.28
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	8	0.28
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	3	0.28
(1,219)	1:3:A:LYS:HD3	1:3:A:LYS:HG2	2	0.28
(1,219)	1:3:A:LYS:HD3	1:3:A:LYS:HG2	9	0.28
(1,212)	1:33:A:ILE:HD11	1:49:A:LYS:HG3	7	0.28
(1,197)	1:45:A:ILE:HG21	1:69:A:ILE:HA	2	0.28
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG23	5	0.28
(1,177)	1:79:A:ILE:HG23	1:110:A:TYR:HB2	1	0.28
(1,169)	1:54:A:ALA:HB3	1:30:A:ILE:HD12	4	0.28
(1,166)	1:34:A:VAL:HG12	1:65:A:ILE:HD13	4	0.28
(1,159)	1:108:A:VAL:HG22	1:34:A:VAL:HA	10	0.28
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	5	0.28
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	7	0.28
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	8	0.28
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	1	0.28
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD23	5	0.28
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	7	0.28
(1,104)	1:3:A:LYS:HE2	1:5:A:SER:HB2	5	0.28
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	5	0.28
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	5	0.28
(1,63)	1:79:A:ILE:HD11	1:62:A:VAL:HG21	8	0.28
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	8	0.28
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	6	0.28
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	10	0.28
(2,1054)	1:107:A:TYR:HD1	1:107:A:TYR:HB2	1	0.27
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	1	0.27
(2,1029)	1:62:A:VAL:HG11	1:77:A:ILE:HG22	7	0.27
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG22	7	0.27
(2,1005)	1:88:A:ALA:HB2	1:62:A:VAL:HG23	7	0.27
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG13	6	0.27
(2,978)	1:81:A:VAL:HG11	1:3:A:LYS:HG2	9	0.27
(2,962)	1:34:A:VAL:HG11	1:45:A:ILE:HG12	3	0.27
(2,959)	1:108:A:VAL:HG23	1:107:A:TYR:HA	1	0.27
(2,959)	1:108:A:VAL:HG21	1:107:A:TYR:HA	8	0.27
(2,959)	1:108:A:VAL:HG21	1:107:A:TYR:HA	9	0.27
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	5	0.27
(2,939)	1:85:A:LEU:HD21	1:85:A:LEU:HD13	3	0.27
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	9	0.27
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	10	0.27
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD12	1	0.27
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD12	4	0.27
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD13	5	0.27
(2,870)	1:42:A:ILE:HD12	1:67:A:LYS:HA	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,870)	1:42:A:ILE:HD11	1:67:A:LYS:HA	4	0.27
(2,870)	1:42:A:ILE:HD11	1:67:A:LYS:HA	5	0.27
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB2	6	0.27
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB3	7	0.27
(2,784)	1:57:A:THR:HG23	1:60:A:GLN:HB2	10	0.27
(2,759)	1:108:A:VAL:HG21	1:108:A:VAL:HA	2	0.27
(2,753)	1:115:A:THR:HG22	1:116:A:PHE:HD2	8	0.27
(2,751)	1:64:A:VAL:HG21	1:61:A:PHE:HD2	1	0.27
(2,751)	1:64:A:VAL:HG22	1:61:A:PHE:HD1	2	0.27
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG11	1	0.27
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG12	6	0.27
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG12	10	0.27
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD12	1	0.27
(2,707)	1:58:A:VAL:HG22	1:57:A:THR:HA	8	0.27
(2,707)	1:58:A:VAL:HG21	1:57:A:THR:HA	10	0.27
(2,705)	1:62:A:VAL:HG22	1:61:A:PHE:HD2	8	0.27
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	10	0.27
(2,695)	1:65:A:ILE:HG13	1:45:A:ILE:HD12	10	0.27
(2,687)	1:16:A:ARG:HG2	1:16:A:ARG:HB2	8	0.27
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	1	0.27
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG12	4	0.27
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG12	7	0.27
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG13	10	0.27
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG13	9	0.27
(2,559)	1:3:A:LYS:HE3	1:81:A:VAL:HG12	6	0.27
(2,535)	1:78:A:PHE:HB3	1:80:A:PHE:HE1	6	0.27
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD21	6	0.27
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD23	9	0.27
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD21	10	0.27
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG13	6	0.27
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG11	3	0.27
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD2	5	0.27
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	3	0.27
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	8	0.27
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	10	0.27
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	6	0.27
(2,150)	1:47:A:LYS:H	1:45:A:ILE:HG21	8	0.27
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	6	0.27
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	9	0.27
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD13	7	0.27
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG21	6	0.27
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG22	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG22	8	0.27
(1,166)	1:34:A:VAL:HG12	1:65:A:ILE:HD13	6	0.27
(1,146)	1:71:A:LEU:HG	1:77:A:ILE:HG23	7	0.27
(1,142)	1:51:A:LEU:HG	1:22:A:ILE:HD13	8	0.27
(1,139)	1:85:A:LEU:HD11	1:78:A:PHE:HE2	10	0.27
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	6	0.27
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD22	2	0.27
(1,104)	1:3:A:LYS:HE3	1:2:A:ALA:HA	2	0.27
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	9	0.27
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD13	10	0.27
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	8	0.27
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HB3	9	0.27
(2,1062)	1:50:A:TYR:HE2	1:64:A:VAL:HG12	8	0.26
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG13	7	0.26
(2,1029)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	4	0.26
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	9	0.26
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG21	2	0.26
(2,987)	1:77:A:ILE:HD11	1:62:A:VAL:HG11	7	0.26
(2,963)	1:62:A:VAL:HG22	1:62:A:VAL:HG23	1	0.26
(2,963)	1:62:A:VAL:HG21	1:62:A:VAL:HG23	6	0.26
(2,959)	1:108:A:VAL:HG22	1:107:A:TYR:HA	4	0.26
(2,959)	1:108:A:VAL:HG22	1:107:A:TYR:HA	7	0.26
(2,908)	1:77:A:ILE:HD11	1:79:A:ILE:HD12	7	0.26
(2,897)	1:79:A:ILE:HD13	1:61:A:PHE:HE2	7	0.26
(2,875)	1:92:A:MET:HE1	1:61:A:PHE:HB3	3	0.26
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB3	1	0.26
(2,804)	1:64:A:VAL:HG22	1:64:A:VAL:HG11	2	0.26
(2,798)	1:109:A:THR:HG22	1:37:A:ALA:HB2	1	0.26
(2,798)	1:109:A:THR:HG22	1:37:A:ALA:HB2	2	0.26
(2,770)	1:115:A:THR:HG23	1:115:A:THR:HA	1	0.26
(2,759)	1:108:A:VAL:HG22	1:108:A:VAL:HA	7	0.26
(2,751)	1:64:A:VAL:HG21	1:61:A:PHE:HD1	3	0.26
(2,751)	1:64:A:VAL:HG23	1:61:A:PHE:HD1	5	0.26
(2,751)	1:64:A:VAL:HG21	1:61:A:PHE:HD1	9	0.26
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG12	3	0.26
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD11	8	0.26
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD11	10	0.26
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG21	1	0.26
(2,707)	1:58:A:VAL:HG21	1:57:A:THR:HA	7	0.26
(2,705)	1:62:A:VAL:HG21	1:61:A:PHE:HD2	2	0.26
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD23	6	0.26
(2,644)	1:113:A:GLU:H	1:113:A:GLU:HB2	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG11	8	0.26
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG12	9	0.26
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG13	6	0.26
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG12	9	0.26
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG13	10	0.26
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD21	3	0.26
(2,515)	1:56:A:LEU:HA	1:91:A:LEU:HD23	5	0.26
(2,483)	1:116:A:PHE:HA	1:116:A:PHE:HD1	8	0.26
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	8	0.26
(2,414)	1:111:A:SER:HB3	1:37:A:ALA:HB3	5	0.26
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD12	8	0.26
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD3	3	0.26
(2,181)	1:100:A:LYS:H	1:100:A:LYS:HG3	9	0.26
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	6	0.26
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	1	0.26
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD12	1	0.26
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD11	2	0.26
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD12	4	0.26
(1,248)	1:50:A:TYR:HE2	1:32:A:VAL:HB	9	0.26
(1,230)	1:57:A:THR:HG22	1:57:A:THR:HA	7	0.26
(1,219)	1:3:A:LYS:HD2	1:3:A:LYS:HG3	1	0.26
(1,219)	1:3:A:LYS:HD3	1:3:A:LYS:HG2	7	0.26
(1,188)	1:54:A:ALA:HB3	1:30:A:ILE:HG13	1	0.26
(1,188)	1:54:A:ALA:HB1	1:30:A:ILE:HG13	8	0.26
(1,188)	1:54:A:ALA:HB1	1:30:A:ILE:HG13	9	0.26
(1,177)	1:79:A:ILE:HG23	1:110:A:TYR:HB2	8	0.26
(1,169)	1:54:A:ALA:HB3	1:30:A:ILE:HD11	6	0.26
(1,166)	1:34:A:VAL:HG12	1:65:A:ILE:HD13	3	0.26
(1,166)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	9	0.26
(1,162)	1:32:A:VAL:HG23	1:106:A:LEU:HB3	1	0.26
(1,154)	1:109:A:THR:HG21	1:37:A:ALA:H	1	0.26
(1,151)	1:51:A:LEU:HD22	1:22:A:ILE:HD13	5	0.26
(1,139)	1:85:A:LEU:HD13	1:78:A:PHE:HE1	4	0.26
(1,139)	1:85:A:LEU:HD12	1:78:A:PHE:HE2	7	0.26
(1,120)	1:113:A:GLU:H	1:113:A:GLU:HG3	3	0.26
(1,120)	1:113:A:GLU:H	1:113:A:GLU:HG3	6	0.26
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD21	8	0.26
(1,114)	1:118:A:PHE:HB2	1:119:A:GLY:HA2	6	0.26
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	1	0.26
(1,92)	1:54:A:ALA:HA	1:30:A:ILE:HD12	2	0.26
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	7	0.26
(1,74)	1:72:A:SER:HB2	1:75:A:LYS:HG3	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	3	0.26
(1,28)	1:60:A:GLN:H	1:56:A:LEU:HD11	2	0.26
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	4	0.26
(1,3)	1:76:A:ALA:H	1:78:A:PHE:HE2	2	0.26
(2,1042)	1:79:A:ILE:HD11	1:79:A:ILE:HD13	1	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD11	2	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD13	3	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD11	4	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD13	5	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD13	6	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD11	7	0.25
(2,1042)	1:79:A:ILE:HD11	1:79:A:ILE:HD13	8	0.25
(2,1042)	1:79:A:ILE:HD11	1:79:A:ILE:HD13	9	0.25
(2,1042)	1:79:A:ILE:HD12	1:79:A:ILE:HD11	10	0.25
(2,1029)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	2	0.25
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG21	1	0.25
(2,1015)	1:79:A:ILE:HG22	1:62:A:VAL:HG22	4	0.25
(2,1007)	1:90:A:ALA:HB1	1:90:A:ALA:HB3	1	0.25
(2,1007)	1:90:A:ALA:HB1	1:90:A:ALA:HB3	2	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB1	3	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB3	4	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB1	5	0.25
(2,1007)	1:90:A:ALA:HB1	1:90:A:ALA:HB3	6	0.25
(2,1007)	1:90:A:ALA:HB1	1:90:A:ALA:HB3	7	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB3	8	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB3	9	0.25
(2,1007)	1:90:A:ALA:HB2	1:90:A:ALA:HB3	10	0.25
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	4	0.25
(2,987)	1:77:A:ILE:HD12	1:62:A:VAL:HG13	8	0.25
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG22	9	0.25
(2,963)	1:62:A:VAL:HG22	1:62:A:VAL:HG23	2	0.25
(2,963)	1:62:A:VAL:HG21	1:62:A:VAL:HG23	3	0.25
(2,963)	1:62:A:VAL:HG21	1:62:A:VAL:HG23	4	0.25
(2,963)	1:62:A:VAL:HG22	1:62:A:VAL:HG23	5	0.25
(2,963)	1:62:A:VAL:HG21	1:62:A:VAL:HG23	7	0.25
(2,963)	1:62:A:VAL:HG21	1:62:A:VAL:HG23	8	0.25
(2,963)	1:62:A:VAL:HG22	1:62:A:VAL:HG21	9	0.25
(2,963)	1:62:A:VAL:HG21	1:62:A:VAL:HG23	10	0.25
(2,962)	1:34:A:VAL:HG12	1:45:A:ILE:HG12	7	0.25
(2,959)	1:108:A:VAL:HG23	1:107:A:TYR:HA	3	0.25
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	4	0.25
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,931)	1:48:A:LYS:HG3	1:47:A:LYS:HE3	2	0.25
(2,931)	1:48:A:LYS:HG3	1:47:A:LYS:HE2	4	0.25
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	7	0.25
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD21	1	0.25
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD22	9	0.25
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD12	2	0.25
(2,908)	1:77:A:ILE:HD13	1:79:A:ILE:HD13	6	0.25
(2,882)	1:45:A:ILE:HG23	1:47:A:LYS:HB3	6	0.25
(2,867)	1:92:A:MET:HE3	1:61:A:PHE:HD2	2	0.25
(2,867)	1:92:A:MET:HE1	1:61:A:PHE:HD2	10	0.25
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD11	8	0.25
(2,822)	1:76:A:ALA:HB2	1:67:A:LYS:HD3	2	0.25
(2,810)	1:76:A:ALA:H	1:76:A:ALA:HB2	8	0.25
(2,804)	1:64:A:VAL:HG22	1:64:A:VAL:HG11	4	0.25
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG13	6	0.25
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG12	8	0.25
(2,800)	1:95:A:VAL:HG22	1:90:A:ALA:HB2	1	0.25
(2,783)	1:109:A:THR:HG22	1:35:A:GLU:HB3	3	0.25
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	6	0.25
(2,759)	1:108:A:VAL:HG23	1:108:A:VAL:HA	1	0.25
(2,759)	1:108:A:VAL:HG23	1:108:A:VAL:HA	3	0.25
(2,759)	1:108:A:VAL:HG22	1:108:A:VAL:HA	4	0.25
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	1	0.25
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	5	0.25
(2,756)	1:57:A:THR:HG23	1:57:A:THR:HA	9	0.25
(2,751)	1:64:A:VAL:HG22	1:61:A:PHE:HD2	4	0.25
(2,751)	1:64:A:VAL:HG21	1:61:A:PHE:HD2	6	0.25
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG13	2	0.25
(2,738)	1:71:A:LEU:HD12	1:77:A:ILE:HG21	2	0.25
(2,738)	1:71:A:LEU:HD13	1:77:A:ILE:HG23	4	0.25
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD13	4	0.25
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD21	8	0.25
(2,708)	1:85:A:LEU:HD21	1:80:A:PHE:HA	6	0.25
(2,702)	1:67:A:LYS:HG2	1:67:A:LYS:H	7	0.25
(2,687)	1:16:A:ARG:HG2	1:16:A:ARG:HB2	7	0.25
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	8	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	1	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	2	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	3	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	4	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	5	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	7	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	8	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	9	0.25
(2,658)	1:27:A:PRO:HB2	1:27:A:PRO:HG3	10	0.25
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	1	0.25
(2,613)	1:13:A:GLU:HG2	1:13:A:GLU:HB3	3	0.25
(2,613)	1:13:A:GLU:HG2	1:13:A:GLU:HB3	6	0.25
(2,613)	1:13:A:GLU:HG2	1:13:A:GLU:HB3	7	0.25
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	9	0.25
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	9	0.25
(2,601)	1:35:A:GLU:HG2	1:33:A:ILE:HG23	4	0.25
(2,555)	1:70:A:LYS:HE3	1:42:A:ILE:HG12	2	0.25
(2,554)	1:39:A:LYS:HE3	1:39:A:LYS:HD2	6	0.25
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB3	8	0.25
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG12	1	0.25
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG12	5	0.25
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG12	8	0.25
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	3	0.25
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	1	0.25
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG21	7	0.25
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD3	6	0.25
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD2	10	0.25
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	2	0.25
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	3	0.25
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD11	6	0.25
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG21	4	0.25
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	1	0.25
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	9	0.25
(1,211)	1:33:A:ILE:HD11	1:49:A:LYS:HD3	8	0.25
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG23	9	0.25
(1,181)	1:22:A:ILE:HG22	1:29:A:ARG:HG3	8	0.25
(1,169)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	2	0.25
(1,166)	1:34:A:VAL:HG12	1:65:A:ILE:HD12	2	0.25
(1,166)	1:34:A:VAL:HG12	1:65:A:ILE:HD12	8	0.25
(1,165)	1:32:A:VAL:HG21	1:32:A:VAL:HG13	9	0.25
(1,154)	1:109:A:THR:HG22	1:37:A:ALA:H	4	0.25
(1,153)	1:32:A:VAL:H	1:52:A:VAL:HG23	6	0.25
(1,152)	1:109:A:THR:HG21	1:80:A:PHE:H	7	0.25
(1,151)	1:51:A:LEU:HD21	1:22:A:ILE:HD12	2	0.25
(1,151)	1:51:A:LEU:HD22	1:22:A:ILE:HD13	6	0.25
(1,139)	1:85:A:LEU:HD13	1:78:A:PHE:HE1	2	0.25
(1,135)	1:53:A:PRO:HB3	1:29:A:ARG:HB3	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD23	1	0.25
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	8	0.25
(1,104)	1:47:A:LYS:HE3	1:5:A:SER:HB2	8	0.25
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	8	0.25
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	4	0.25
(2,1062)	1:50:A:TYR:HE1	1:64:A:VAL:HG12	7	0.24
(2,1048)	1:54:A:ALA:HB1	1:30:A:ILE:HD13	8	0.24
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG11	4	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	1	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	2	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG21	3	0.24
(2,1018)	1:79:A:ILE:HG21	1:79:A:ILE:HG23	5	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	6	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	7	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	8	0.24
(2,1018)	1:79:A:ILE:HG21	1:79:A:ILE:HG23	9	0.24
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	10	0.24
(2,1005)	1:88:A:ALA:HB1	1:62:A:VAL:HG23	4	0.24
(2,1005)	1:88:A:ALA:HB3	1:62:A:VAL:HG23	6	0.24
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	5	0.24
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	9	0.24
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	10	0.24
(2,987)	1:77:A:ILE:HD13	1:62:A:VAL:HG12	5	0.24
(2,982)	1:95:A:VAL:HG22	1:95:A:VAL:HG21	1	0.24
(2,982)	1:95:A:VAL:HG21	1:95:A:VAL:HG23	2	0.24
(2,982)	1:95:A:VAL:HG22	1:95:A:VAL:HG21	3	0.24
(2,982)	1:95:A:VAL:HG21	1:95:A:VAL:HG23	4	0.24
(2,982)	1:95:A:VAL:HG21	1:95:A:VAL:HG23	5	0.24
(2,982)	1:95:A:VAL:HG22	1:95:A:VAL:HG21	6	0.24
(2,982)	1:95:A:VAL:HG21	1:95:A:VAL:HG23	7	0.24
(2,982)	1:95:A:VAL:HG22	1:95:A:VAL:HG23	8	0.24
(2,982)	1:95:A:VAL:HG21	1:95:A:VAL:HG23	9	0.24
(2,982)	1:95:A:VAL:HG21	1:95:A:VAL:HG23	10	0.24
(2,978)	1:81:A:VAL:HG13	1:3:A:LYS:HG3	10	0.24
(2,973)	1:70:A:LYS:HE2	1:115:A:THR:HG23	6	0.24
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG23	8	0.24
(2,959)	1:108:A:VAL:HG21	1:107:A:TYR:HA	6	0.24
(2,959)	1:108:A:VAL:HG23	1:107:A:TYR:HA	10	0.24
(2,945)	1:25:A:LYS:HE3	1:25:A:LYS:HG3	10	0.24
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG21	5	0.24
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	1	0.24
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,892)	1:69:A:ILE:HG23	1:69:A:ILE:HD11	1	0.24
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB3	3	0.24
(2,804)	1:64:A:VAL:HG23	1:64:A:VAL:HG13	5	0.24
(2,798)	1:109:A:THR:HG21	1:37:A:ALA:HB3	10	0.24
(2,786)	1:12:A:LEU:HD11	1:16:A:ARG:HB2	2	0.24
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	5	0.24
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	2	0.24
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG11	9	0.24
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG11	10	0.24
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD13	7	0.24
(2,707)	1:58:A:VAL:HG23	1:57:A:THR:HA	5	0.24
(2,687)	1:16:A:ARG:HG2	1:16:A:ARG:HB2	10	0.24
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD22	8	0.24
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	9	0.24
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	2	0.24
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	5	0.24
(2,578)	1:82:A:ASP:HB3	1:84:A:VAL:HG11	1	0.24
(2,557)	1:39:A:LYS:HE3	1:39:A:LYS:HG2	4	0.24
(2,557)	1:39:A:LYS:HE3	1:39:A:LYS:HG2	10	0.24
(2,554)	1:39:A:LYS:HE3	1:39:A:LYS:HD2	9	0.24
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB3	7	0.24
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	2	0.24
(2,520)	1:87:A:PRO:HD3	1:58:A:VAL:HG11	2	0.24
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG21	1	0.24
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	1	0.24
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	4	0.24
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	10	0.24
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	1	0.24
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD11	4	0.24
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	2	0.24
(2,282)	1:66:A:ARG:H	1:65:A:ILE:HG23	9	0.24
(2,181)	1:100:A:LYS:H	1:100:A:LYS:HG3	2	0.24
(2,113)	1:92:A:MET:H	1:57:A:THR:HG21	3	0.24
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG21	3	0.24
(1,209)	1:30:A:ILE:HD11	1:106:A:LEU:HB2	8	0.24
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG21	4	0.24
(1,182)	1:30:A:ILE:HG23	1:32:A:VAL:HB	9	0.24
(1,169)	1:54:A:ALA:HB2	1:30:A:ILE:HD12	5	0.24
(1,166)	1:34:A:VAL:HG13	1:65:A:ILE:HD13	1	0.24
(1,165)	1:32:A:VAL:HG22	1:32:A:VAL:HG13	8	0.24
(1,165)	1:32:A:VAL:HG22	1:32:A:VAL:HG13	10	0.24
(1,159)	1:108:A:VAL:HG22	1:34:A:VAL:HA	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG21	2	0.24
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG21	5	0.24
(1,122)	1:113:A:GLU:HG2	1:113:A:GLU:HA	9	0.24
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD21	7	0.24
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	10	0.24
(1,77)	1:94:A:SER:HB3	1:98:A:GLU:HB2	6	0.24
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	6	0.24
(2,1046)	1:79:A:ILE:HD11	1:108:A:VAL:HG11	5	0.23
(2,1033)	1:69:A:ILE:HG21	1:65:A:ILE:HG23	3	0.23
(2,1018)	1:79:A:ILE:HG22	1:79:A:ILE:HG23	4	0.23
(2,1017)	1:79:A:ILE:HG23	1:108:A:VAL:HG12	10	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	1	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	2	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	3	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	4	0.23
(2,995)	1:64:A:VAL:HG12	1:64:A:VAL:HG11	5	0.23
(2,995)	1:64:A:VAL:HG12	1:64:A:VAL:HG13	6	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	7	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	8	0.23
(2,995)	1:64:A:VAL:HG11	1:64:A:VAL:HG13	9	0.23
(2,995)	1:64:A:VAL:HG12	1:64:A:VAL:HG11	10	0.23
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	7	0.23
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	8	0.23
(2,978)	1:81:A:VAL:HG11	1:3:A:LYS:HG3	5	0.23
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG22	1	0.23
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	3	0.23
(2,931)	1:48:A:LYS:HG3	1:47:A:LYS:HE2	5	0.23
(2,899)	1:65:A:ILE:HD12	1:61:A:PHE:HE2	10	0.23
(2,888)	1:92:A:MET:HE3	1:108:A:VAL:HG23	4	0.23
(2,888)	1:92:A:MET:HE3	1:108:A:VAL:HG22	8	0.23
(2,875)	1:92:A:MET:HE3	1:61:A:PHE:HB3	7	0.23
(2,870)	1:42:A:ILE:HD11	1:67:A:LYS:HA	9	0.23
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB2	1	0.23
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB3	4	0.23
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB2	8	0.23
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB2	9	0.23
(2,823)	1:76:A:ALA:HB3	1:77:A:ILE:HG22	10	0.23
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG12	3	0.23
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG11	9	0.23
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	8	0.23
(2,783)	1:109:A:THR:HG23	1:35:A:GLU:HB3	7	0.23
(2,764)	1:109:A:THR:HG21	1:37:A:ALA:HA	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	10	0.23
(2,756)	1:57:A:THR:HG22	1:57:A:THR:HA	7	0.23
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG13	2	0.23
(2,741)	1:59:A:GLY:H	1:58:A:VAL:HG11	9	0.23
(2,737)	1:71:A:LEU:HG	1:71:A:LEU:HD12	2	0.23
(2,724)	1:51:A:LEU:HD22	1:29:A:ARG:HB2	3	0.23
(2,724)	1:51:A:LEU:HD22	1:29:A:ARG:HB2	9	0.23
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	1	0.23
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	9	0.23
(2,708)	1:85:A:LEU:HD23	1:80:A:PHE:HA	1	0.23
(2,708)	1:85:A:LEU:HD21	1:80:A:PHE:HA	9	0.23
(2,687)	1:16:A:ARG:HG2	1:16:A:ARG:HB2	5	0.23
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD23	10	0.23
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	1	0.23
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	3	0.23
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	6	0.23
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	7	0.23
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	10	0.23
(2,644)	1:113:A:GLU:H	1:113:A:GLU:HB2	2	0.23
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	4	0.23
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG22	8	0.23
(2,557)	1:39:A:LYS:HE3	1:39:A:LYS:HG2	2	0.23
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	5	0.23
(2,535)	1:78:A:PHE:HB2	1:80:A:PHE:HE2	9	0.23
(2,485)	1:116:A:PHE:HA	1:116:A:PHE:HB2	1	0.23
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG12	9	0.23
(2,399)	1:65:A:ILE:HG23	1:77:A:ILE:HD11	2	0.23
(2,399)	1:65:A:ILE:HG21	1:77:A:ILE:HD11	9	0.23
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB1	7	0.23
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD2	9	0.23
(2,219)	1:49:A:LYS:H	1:48:A:LYS:HB3	3	0.23
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	1	0.23
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	5	0.23
(2,181)	1:100:A:LYS:H	1:100:A:LYS:HG3	1	0.23
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD13	4	0.23
(2,19)	1:34:A:VAL:H	1:33:A:ILE:HD12	9	0.23
(1,230)	1:109:A:THR:HG21	1:109:A:THR:HA	1	0.23
(1,196)	1:45:A:ILE:HA	1:45:A:ILE:HG21	9	0.23
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG22	1	0.23
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG21	2	0.23
(1,178)	1:33:A:ILE:HG21	1:6:A:PHE:HB3	6	0.23
(1,177)	1:79:A:ILE:HG23	1:110:A:TYR:HB2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:79:A:ILE:HG23	1:110:A:TYR:HB2	9	0.23
(1,172)	1:30:A:ILE:HG22	1:52:A:VAL:H	5	0.23
(1,169)	1:54:A:ALA:HB3	1:30:A:ILE:HD12	1	0.23
(1,166)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	5	0.23
(1,159)	1:108:A:VAL:HG23	1:34:A:VAL:HA	9	0.23
(1,151)	1:51:A:LEU:HD22	1:22:A:ILE:HD11	4	0.23
(1,151)	1:51:A:LEU:HD21	1:22:A:ILE:HD12	9	0.23
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD23	4	0.23
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD23	6	0.23
(1,117)	1:22:A:ILE:HB	1:51:A:LEU:HD22	9	0.23
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	3	0.23
(1,74)	1:72:A:SER:HB2	1:75:A:LYS:HG2	5	0.23
(1,53)	1:99:A:LYS:H	1:98:A:GLU:HG2	10	0.23
(1,38)	1:113:A:GLU:H	1:113:A:GLU:HB3	5	0.23
(1,29)	1:109:A:THR:H	1:110:A:TYR:H	10	0.23
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	10	0.22
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	4	0.22
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG11	1	0.22
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG11	2	0.22
(2,1033)	1:69:A:ILE:HG23	1:65:A:ILE:HG21	5	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG23	1	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG23	2	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	3	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	4	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	5	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	6	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	7	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	8	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG23	9	0.22
(2,1031)	1:77:A:ILE:HG22	1:77:A:ILE:HG21	10	0.22
(2,990)	1:81:A:VAL:HG22	1:80:A:PHE:HA	1	0.22
(2,990)	1:81:A:VAL:HG23	1:80:A:PHE:HA	2	0.22
(2,990)	1:81:A:VAL:HG21	1:80:A:PHE:HA	3	0.22
(2,990)	1:81:A:VAL:HG22	1:80:A:PHE:HA	6	0.22
(2,986)	1:62:A:VAL:HG11	1:62:A:VAL:HG13	1	0.22
(2,986)	1:62:A:VAL:HG11	1:62:A:VAL:HG13	2	0.22
(2,986)	1:62:A:VAL:HG12	1:62:A:VAL:HG13	3	0.22
(2,986)	1:62:A:VAL:HG12	1:62:A:VAL:HG13	4	0.22
(2,986)	1:62:A:VAL:HG12	1:62:A:VAL:HG13	5	0.22
(2,986)	1:62:A:VAL:HG11	1:62:A:VAL:HG13	6	0.22
(2,986)	1:62:A:VAL:HG12	1:62:A:VAL:HG11	7	0.22
(2,986)	1:62:A:VAL:HG11	1:62:A:VAL:HG13	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,986)	1:62:A:VAL:HG11	1:62:A:VAL:HG13	9	0.22
(2,986)	1:62:A:VAL:HG12	1:62:A:VAL:HG11	10	0.22
(2,962)	1:34:A:VAL:HG12	1:45:A:ILE:HG12	9	0.22
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	3	0.22
(2,952)	1:51:A:LEU:HD11	1:51:A:LEU:HD13	1	0.22
(2,952)	1:51:A:LEU:HD11	1:51:A:LEU:HD13	2	0.22
(2,952)	1:51:A:LEU:HD11	1:51:A:LEU:HD13	3	0.22
(2,952)	1:51:A:LEU:HD12	1:51:A:LEU:HD11	4	0.22
(2,952)	1:51:A:LEU:HD11	1:51:A:LEU:HD13	5	0.22
(2,952)	1:51:A:LEU:HD12	1:51:A:LEU:HD13	6	0.22
(2,952)	1:51:A:LEU:HD12	1:51:A:LEU:HD13	7	0.22
(2,952)	1:51:A:LEU:HD11	1:51:A:LEU:HD13	8	0.22
(2,952)	1:51:A:LEU:HD11	1:51:A:LEU:HD13	9	0.22
(2,952)	1:51:A:LEU:HD12	1:51:A:LEU:HD13	10	0.22
(2,948)	1:71:A:LEU:HD21	1:71:A:LEU:HD23	9	0.22
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG22	4	0.22
(2,905)	1:79:A:ILE:HD11	1:62:A:VAL:HG22	8	0.22
(2,888)	1:92:A:MET:HE2	1:108:A:VAL:HG21	1	0.22
(2,888)	1:92:A:MET:HE1	1:108:A:VAL:HG22	9	0.22
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD13	2	0.22
(2,846)	1:33:A:ILE:HG21	1:35:A:GLU:HG3	1	0.22
(2,808)	1:32:A:VAL:HG23	1:32:A:VAL:HG11	5	0.22
(2,805)	1:44:A:THR:HG21	1:45:A:ILE:HG22	4	0.22
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	5	0.22
(2,783)	1:109:A:THR:HG22	1:35:A:GLU:HB3	6	0.22
(2,770)	1:115:A:THR:HG22	1:115:A:THR:HA	3	0.22
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	1	0.22
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	3	0.22
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	6	0.22
(2,744)	1:109:A:THR:H	1:108:A:VAL:HG13	5	0.22
(2,724)	1:51:A:LEU:HD22	1:29:A:ARG:HB2	2	0.22
(2,724)	1:51:A:LEU:HD23	1:29:A:ARG:HB2	4	0.22
(2,724)	1:51:A:LEU:HD21	1:29:A:ARG:HB2	7	0.22
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	2	0.22
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	4	0.22
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	5	0.22
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	8	0.22
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	8	0.22
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG12	6	0.22
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG22	5	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	1	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	3	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	5	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	6	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	7	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	8	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	9	0.22
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	10	0.22
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG12	3	0.22
(2,453)	1:69:A:ILE:HA	1:69:A:ILE:HG13	2	0.22
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	9	0.22
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD13	2	0.22
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD13	4	0.22
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD11	3	0.22
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD12	7	0.22
(2,399)	1:65:A:ILE:HG21	1:77:A:ILE:HD13	8	0.22
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB3	4	0.22
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB1	8	0.22
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	6	0.22
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG12	5	0.22
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG13	10	0.22
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	9	0.22
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB2	1	0.22
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	4	0.22
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	4	0.22
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	8	0.22
(2,26)	1:32:A:VAL:H	1:32:A:VAL:HG11	3	0.22
(1,230)	1:57:A:THR:HG21	1:57:A:THR:HA	8	0.22
(1,229)	1:32:A:VAL:HG21	1:32:A:VAL:HG23	1	0.22
(1,229)	1:52:A:VAL:HG22	1:52:A:VAL:HG23	2	0.22
(1,229)	1:52:A:VAL:HG22	1:52:A:VAL:HG21	3	0.22
(1,229)	1:52:A:VAL:HG22	1:52:A:VAL:HG21	4	0.22
(1,229)	1:52:A:VAL:HG21	1:52:A:VAL:HG23	5	0.22
(1,229)	1:52:A:VAL:HG21	1:52:A:VAL:HG23	6	0.22
(1,229)	1:32:A:VAL:HG21	1:32:A:VAL:HG23	7	0.22
(1,229)	1:32:A:VAL:HG21	1:32:A:VAL:HG23	8	0.22
(1,229)	1:52:A:VAL:HG22	1:52:A:VAL:HG23	9	0.22
(1,229)	1:32:A:VAL:HG21	1:32:A:VAL:HG23	10	0.22
(1,212)	1:33:A:ILE:HD13	1:49:A:LYS:HG2	9	0.22
(1,211)	1:33:A:ILE:HD12	1:49:A:LYS:HD3	6	0.22
(1,197)	1:45:A:ILE:HG22	1:69:A:ILE:HA	8	0.22
(1,169)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	3	0.22
(1,169)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:108:A:VAL:HG23	1:34:A:VAL:HA	8	0.22
(1,153)	1:32:A:VAL:H	1:32:A:VAL:HG21	2	0.22
(1,151)	1:51:A:LEU:HD22	1:22:A:ILE:HD11	3	0.22
(1,150)	1:71:A:LEU:HD11	1:42:A:ILE:HG13	4	0.22
(1,139)	1:85:A:LEU:HD12	1:78:A:PHE:HE1	5	0.22
(1,139)	1:85:A:LEU:HD13	1:78:A:PHE:HE1	6	0.22
(1,110)	1:110:A:TYR:HB3	1:34:A:VAL:HG22	3	0.22
(1,73)	1:62:A:VAL:HA	1:77:A:ILE:HG13	9	0.22
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	10	0.22
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	8	0.22
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG11	10	0.22
(1,29)	1:109:A:THR:H	1:110:A:TYR:H	5	0.22
(1,29)	1:109:A:THR:H	1:110:A:TYR:H	6	0.22
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG21	6	0.22
(3,51)	1:33:A:ILE:N	1:106:A:LEU:O	10	0.21
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	3	0.21
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	1	0.21
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE2	5	0.21
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG12	9	0.21
(2,978)	1:81:A:VAL:HG12	1:3:A:LYS:HG3	4	0.21
(2,960)	1:110:A:TYR:HB3	1:34:A:VAL:HG12	4	0.21
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG21	6	0.21
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	5	0.21
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	9	0.21
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	10	0.21
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	4	0.21
(2,905)	1:79:A:ILE:HD11	1:62:A:VAL:HG22	3	0.21
(2,888)	1:92:A:MET:HE1	1:108:A:VAL:HG21	10	0.21
(2,869)	1:92:A:MET:HE3	1:58:A:VAL:HA	1	0.21
(2,867)	1:92:A:MET:HE3	1:61:A:PHE:HD1	4	0.21
(2,856)	1:79:A:ILE:HG12	1:79:A:ILE:HG22	9	0.21
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB3	6	0.21
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB2	7	0.21
(2,804)	1:64:A:VAL:HG22	1:64:A:VAL:HG12	7	0.21
(2,804)	1:64:A:VAL:HG23	1:64:A:VAL:HG13	10	0.21
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	1	0.21
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	3	0.21
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	10	0.21
(2,783)	1:109:A:THR:HG21	1:35:A:GLU:HB3	9	0.21
(2,780)	1:115:A:THR:HG23	1:116:A:PHE:HB3	3	0.21
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG21	6	0.21
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,762)	1:57:A:THR:HG21	1:56:A:LEU:HA	7	0.21
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	8	0.21
(2,762)	1:57:A:THR:HG22	1:56:A:LEU:HA	9	0.21
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	10	0.21
(2,731)	1:85:A:LEU:HB3	1:85:A:LEU:HD22	9	0.21
(2,724)	1:51:A:LEU:HD23	1:29:A:ARG:HB2	1	0.21
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	3	0.21
(2,720)	1:78:A:PHE:HB3	1:85:A:LEU:HD21	4	0.21
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	1	0.21
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	2	0.21
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	5	0.21
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	6	0.21
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	7	0.21
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	8	0.21
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	10	0.21
(2,708)	1:85:A:LEU:HD21	1:80:A:PHE:HA	10	0.21
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD21	4	0.21
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD22	5	0.21
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	2	0.21
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	4	0.21
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	7	0.21
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG2	4	0.21
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	2	0.21
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	4	0.21
(2,644)	1:113:A:GLU:H	1:113:A:GLU:HB2	7	0.21
(2,619)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	8	0.21
(2,613)	1:13:A:GLU:HG3	1:13:A:GLU:HB2	10	0.21
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	7	0.21
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	2	0.21
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG13	7	0.21
(2,555)	1:70:A:LYS:HE2	1:42:A:ILE:HG12	6	0.21
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG21	2	0.21
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG11	1	0.21
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD13	1	0.21
(2,399)	1:65:A:ILE:HG23	1:77:A:ILE:HD11	1	0.21
(2,382)	1:55:A:ASP:H	1:55:A:ASP:HB3	10	0.21
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	5	0.21
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG12	4	0.21
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD3	2	0.21
(2,184)	1:71:A:LEU:H	1:69:A:ILE:HG13	2	0.21
(2,150)	1:47:A:LYS:H	1:45:A:ILE:HG23	4	0.21
(2,150)	1:47:A:LYS:H	1:45:A:ILE:HG23	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	5	0.21
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	5	0.21
(2,62)	1:101:A:ASP:H	1:101:A:ASP:HB2	7	0.21
(1,206)	1:65:A:ILE:HD13	1:34:A:VAL:HG21	4	0.21
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG23	7	0.21
(1,182)	1:30:A:ILE:HG22	1:32:A:VAL:HB	2	0.21
(1,182)	1:30:A:ILE:HG22	1:32:A:VAL:HB	5	0.21
(1,178)	1:33:A:ILE:HG22	1:6:A:PHE:HB2	3	0.21
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB1	1	0.21
(1,172)	1:30:A:ILE:HG23	1:52:A:VAL:H	4	0.21
(1,172)	1:30:A:ILE:HG22	1:52:A:VAL:H	10	0.21
(1,163)	1:64:A:VAL:HG21	1:52:A:VAL:HB	8	0.21
(1,159)	1:108:A:VAL:HG23	1:34:A:VAL:HA	6	0.21
(1,141)	1:87:A:PRO:HG2	1:95:A:VAL:HG21	7	0.21
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	3	0.21
(1,78)	1:39:A:LYS:H	1:38:A:GLU:HA	1	0.21
(1,78)	1:39:A:LYS:H	1:38:A:GLU:HA	7	0.21
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HD2	2	0.21
(1,51)	1:67:A:LYS:H	1:67:A:LYS:HD2	8	0.21
(1,29)	1:109:A:THR:H	1:110:A:TYR:H	9	0.21
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	5	0.2
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	7	0.2
(2,1054)	1:107:A:TYR:HD1	1:107:A:TYR:HB2	3	0.2
(2,1048)	1:54:A:ALA:HB3	1:30:A:ILE:HD12	4	0.2
(2,1046)	1:79:A:ILE:HD11	1:108:A:VAL:HG13	6	0.2
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG12	10	0.2
(2,1017)	1:79:A:ILE:HG23	1:108:A:VAL:HG12	3	0.2
(2,973)	1:70:A:LYS:HE2	1:115:A:THR:HG23	7	0.2
(2,962)	1:34:A:VAL:HG12	1:45:A:ILE:HG12	5	0.2
(2,948)	1:71:A:LEU:HD21	1:71:A:LEU:HD23	1	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD23	2	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD23	3	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD23	4	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD21	5	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD21	6	0.2
(2,948)	1:71:A:LEU:HD21	1:71:A:LEU:HD23	7	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD21	8	0.2
(2,948)	1:71:A:LEU:HD22	1:71:A:LEU:HD21	10	0.2
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	1	0.2
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	6	0.2
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD12	7	0.2
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	6	0.2
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	7	0.2
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG23	9	0.2
(2,901)	1:79:A:ILE:HD11	1:79:A:ILE:HB	5	0.2
(2,888)	1:92:A:MET:HE2	1:108:A:VAL:HG22	5	0.2
(2,870)	1:42:A:ILE:HD11	1:67:A:LYS:HA	2	0.2
(2,869)	1:92:A:MET:HE3	1:58:A:VAL:HA	6	0.2
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD12	7	0.2
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB1	2	0.2
(2,823)	1:76:A:ALA:HB1	1:77:A:ILE:HG22	4	0.2
(2,823)	1:76:A:ALA:HB2	1:77:A:ILE:HG22	5	0.2
(2,804)	1:64:A:VAL:HG21	1:64:A:VAL:HG12	1	0.2
(2,798)	1:109:A:THR:HG23	1:37:A:ALA:HB3	4	0.2
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	2	0.2
(2,793)	1:57:A:THR:HG22	1:56:A:LEU:HB2	9	0.2
(2,783)	1:109:A:THR:HG21	1:35:A:GLU:HB3	2	0.2
(2,779)	1:109:A:THR:HG22	1:80:A:PHE:HB2	2	0.2
(2,751)	1:64:A:VAL:HG23	1:61:A:PHE:HD1	10	0.2
(2,730)	1:71:A:LEU:HD11	1:67:A:LYS:HB2	3	0.2
(2,727)	1:12:A:LEU:HD22	1:16:A:ARG:HG2	2	0.2
(2,722)	1:98:A:GLU:HB2	1:99:A:LYS:HG2	6	0.2
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	9	0.2
(2,691)	1:85:A:LEU:HD11	1:85:A:LEU:HB2	3	0.2
(2,684)	1:21:A:ARG:HG3	1:21:A:ARG:HA	10	0.2
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	6	0.2
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	4	0.2
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG21	10	0.2
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	4	0.2
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	7	0.2
(2,487)	1:74:A:GLU:HA	1:74:A:GLU:HG3	6	0.2
(2,444)	1:15:A:ARG:HA	1:18:A:GLU:HB3	5	0.2
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	6	0.2
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD13	7	0.2
(2,399)	1:65:A:ILE:HG22	1:77:A:ILE:HD11	6	0.2
(2,367)	1:40:A:SER:H	1:37:A:ALA:HB2	10	0.2
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	8	0.2
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG11	8	0.2
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB2	6	0.2
(2,176)	1:17:A:ALA:H	1:16:A:ARG:HB3	10	0.2
(2,151)	1:56:A:LEU:H	1:91:A:LEU:HD13	3	0.2
(2,77)	1:61:A:PHE:H	1:56:A:LEU:HD11	4	0.2
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD1	10	0.2
(2,10)	1:85:A:LEU:H	1:80:A:PHE:HD1	9	0.2
(1,238)	1:69:A:ILE:HG23	1:45:A:ILE:HA	6	0.2
(1,230)	1:57:A:THR:HG21	1:57:A:THR:HA	3	0.2
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG21	4	0.2
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG21	5	0.2
(1,178)	1:33:A:ILE:HG22	1:6:A:PHE:HB2	1	0.2
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB1	6	0.2
(1,172)	1:30:A:ILE:HG22	1:52:A:VAL:H	1	0.2
(1,172)	1:30:A:ILE:HG22	1:52:A:VAL:H	2	0.2
(1,172)	1:30:A:ILE:HG23	1:52:A:VAL:H	8	0.2
(1,172)	1:30:A:ILE:HG23	1:52:A:VAL:H	9	0.2
(1,167)	1:65:A:ILE:HD12	1:34:A:VAL:HG21	7	0.2
(1,159)	1:108:A:VAL:HG22	1:34:A:VAL:HA	1	0.2
(1,150)	1:71:A:LEU:HD13	1:42:A:ILE:HG13	1	0.2
(1,136)	1:29:A:ARG:HG2	1:22:A:ILE:HD11	3	0.2
(1,130)	1:3:A:LYS:HB2	1:3:A:LYS:HG2	1	0.2
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	6	0.2
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	10	0.2
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	1	0.2
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	9	0.2
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	4	0.19
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	5	0.19
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	1	0.19
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	4	0.19
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	9	0.19
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	10	0.19
(2,1005)	1:88:A:ALA:HB2	1:62:A:VAL:HG23	10	0.19
(2,976)	1:115:A:THR:HG22	1:70:A:LYS:HD2	9	0.19
(2,962)	1:34:A:VAL:HG12	1:45:A:ILE:HG12	1	0.19
(2,962)	1:34:A:VAL:HG11	1:45:A:ILE:HG12	6	0.19
(2,959)	1:108:A:VAL:HG21	1:107:A:TYR:HA	5	0.19
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	7	0.19
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	2	0.19
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG2	7	0.19
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD22	5	0.19
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD23	6	0.19
(2,888)	1:92:A:MET:HE2	1:108:A:VAL:HG22	6	0.19
(2,871)	1:112:A:GLY:HA2	1:42:A:ILE:HD11	6	0.19
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD11	6	0.19
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB3	9	0.19
(2,796)	1:32:A:VAL:HG13	1:32:A:VAL:HB	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,793)	1:57:A:THR:HG23	1:56:A:LEU:HB2	6	0.19
(2,770)	1:115:A:THR:HG21	1:115:A:THR:HA	4	0.19
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	8	0.19
(2,727)	1:12:A:LEU:HD21	1:16:A:ARG:HG2	1	0.19
(2,727)	1:12:A:LEU:HD22	1:16:A:ARG:HG2	4	0.19
(2,724)	1:51:A:LEU:HD23	1:29:A:ARG:HB2	6	0.19
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD12	7	0.19
(2,708)	1:85:A:LEU:HD22	1:80:A:PHE:HA	4	0.19
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	5	0.19
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	8	0.19
(2,636)	1:8:A:GLN:HG2	1:9:A:GLU:HB2	4	0.19
(2,557)	1:39:A:LYS:HE3	1:39:A:LYS:HG2	5	0.19
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	10	0.19
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB1	4	0.19
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	8	0.19
(2,498)	1:9:A:GLU:HA	1:9:A:GLU:HB3	4	0.19
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	1	0.19
(2,487)	1:74:A:GLU:HA	1:74:A:GLU:HG3	2	0.19
(2,487)	1:74:A:GLU:HA	1:74:A:GLU:HG3	8	0.19
(2,487)	1:74:A:GLU:HA	1:74:A:GLU:HG3	9	0.19
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG11	2	0.19
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	8	0.19
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB1	3	0.19
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB2	5	0.19
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	1	0.19
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	4	0.19
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	7	0.19
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	10	0.19
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB3	4	0.19
(2,146)	1:75:A:LYS:H	1:75:A:LYS:HG2	4	0.19
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	9	0.19
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	7	0.19
(2,3)	1:37:A:ALA:H	1:36:A:LYS:HB3	10	0.19
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG21	8	0.19
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	5	0.19
(1,201)	1:22:A:ILE:HD13	1:51:A:LEU:HD13	5	0.19
(1,201)	1:22:A:ILE:HD13	1:51:A:LEU:HD11	6	0.19
(1,201)	1:22:A:ILE:HD12	1:51:A:LEU:HD11	7	0.19
(1,183)	1:51:A:LEU:HG	1:22:A:ILE:HG21	6	0.19
(1,178)	1:33:A:ILE:HG22	1:6:A:PHE:HB2	9	0.19
(1,162)	1:32:A:VAL:HG21	1:106:A:LEU:HB3	6	0.19
(1,159)	1:108:A:VAL:HG21	1:34:A:VAL:HA	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:108:A:VAL:HG23	1:34:A:VAL:HA	5	0.19
(1,153)	1:32:A:VAL:H	1:52:A:VAL:HG22	4	0.19
(1,151)	1:51:A:LEU:HD23	1:22:A:ILE:HD12	7	0.19
(1,150)	1:71:A:LEU:HD12	1:42:A:ILE:HG13	3	0.19
(1,150)	1:71:A:LEU:HD13	1:42:A:ILE:HG13	5	0.19
(1,139)	1:85:A:LEU:HD11	1:78:A:PHE:HE2	1	0.19
(1,127)	1:3:A:LYS:HB3	1:109:A:THR:HB	8	0.19
(1,126)	1:76:A:ALA:H	1:75:A:LYS:HB3	5	0.19
(1,115)	1:61:A:PHE:HB3	1:56:A:LEU:HD12	3	0.19
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	5	0.19
(1,105)	1:80:A:PHE:HB2	1:109:A:THR:HB	6	0.19
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB3	8	0.19
(1,68)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	3	0.19
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG21	10	0.19
(1,9)	1:108:A:VAL:H	1:107:A:TYR:HE2	4	0.19
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	7	0.18
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	8	0.18
(2,1048)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	2	0.18
(2,1048)	1:54:A:ALA:HB3	1:30:A:ILE:HD11	6	0.18
(2,1046)	1:79:A:ILE:HD13	1:108:A:VAL:HG12	9	0.18
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG22	5	0.18
(2,978)	1:81:A:VAL:HG11	1:3:A:LYS:HG2	7	0.18
(2,974)	1:115:A:THR:HG22	1:116:A:PHE:HB3	4	0.18
(2,973)	1:70:A:LYS:HE3	1:115:A:THR:HG23	5	0.18
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	6	0.18
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	10	0.18
(2,954)	1:12:A:LEU:HD22	1:12:A:LEU:HD11	7	0.18
(2,938)	1:71:A:LEU:HD11	1:115:A:THR:HG23	9	0.18
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	1	0.18
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	6	0.18
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD21	3	0.18
(2,901)	1:79:A:ILE:HD11	1:79:A:ILE:HB	6	0.18
(2,819)	1:73:A:ALA:HB3	1:74:A:GLU:HB2	7	0.18
(2,808)	1:32:A:VAL:HG21	1:32:A:VAL:HG11	4	0.18
(2,800)	1:95:A:VAL:HG21	1:90:A:ALA:HB3	9	0.18
(2,796)	1:32:A:VAL:HG13	1:32:A:VAL:HB	2	0.18
(2,796)	1:32:A:VAL:HG13	1:32:A:VAL:HB	5	0.18
(2,796)	1:32:A:VAL:HG11	1:32:A:VAL:HB	6	0.18
(2,793)	1:57:A:THR:HG21	1:56:A:LEU:HB2	7	0.18
(2,791)	1:95:A:VAL:HG21	1:95:A:VAL:HB	7	0.18
(2,784)	1:57:A:THR:HG23	1:60:A:GLN:HB2	5	0.18
(2,753)	1:115:A:THR:HG22	1:116:A:PHE:HD2	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD22	4	0.18
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD21	10	0.18
(2,730)	1:71:A:LEU:HD12	1:67:A:LYS:HB3	2	0.18
(2,726)	1:67:A:LYS:HG2	1:67:A:LYS:HD3	2	0.18
(2,724)	1:51:A:LEU:HD23	1:29:A:ARG:HB2	5	0.18
(2,677)	1:85:A:LEU:HD12	1:78:A:PHE:HD1	9	0.18
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	1	0.18
(2,671)	1:70:A:LYS:HD2	1:70:A:LYS:HG3	3	0.18
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	5	0.18
(2,644)	1:113:A:GLU:H	1:113:A:GLU:HB2	5	0.18
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	5	0.18
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	9	0.18
(2,619)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	1	0.18
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	5	0.18
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	10	0.18
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	4	0.18
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	7	0.18
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	4	0.18
(2,513)	1:20:A:ALA:HA	1:23:A:ARG:HG2	8	0.18
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG21	9	0.18
(2,493)	1:23:A:ARG:HA	1:23:A:ARG:HG2	4	0.18
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG22	4	0.18
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG22	5	0.18
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG12	8	0.18
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG11	10	0.18
(2,433)	1:40:A:SER:HB2	1:37:A:ALA:HB2	5	0.18
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	9	0.18
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	6	0.18
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB1	2	0.18
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB2	3	0.18
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	1	0.18
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	5	0.18
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	8	0.18
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD2	2	0.18
(1,230)	1:109:A:THR:HG21	1:109:A:THR:HA	2	0.18
(1,230)	1:109:A:THR:HG21	1:109:A:THR:HA	9	0.18
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	6	0.18
(1,201)	1:22:A:ILE:HD11	1:51:A:LEU:HD13	4	0.18
(1,197)	1:45:A:ILE:HG22	1:69:A:ILE:HA	4	0.18
(1,188)	1:54:A:ALA:HB1	1:30:A:ILE:HG13	3	0.18
(1,172)	1:30:A:ILE:HG23	1:52:A:VAL:H	7	0.18
(1,162)	1:32:A:VAL:HG21	1:106:A:LEU:HB3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:108:A:VAL:HG23	1:34:A:VAL:HA	2	0.18
(1,156)	1:34:A:VAL:HG13	1:110:A:TYR:H	4	0.18
(1,151)	1:51:A:LEU:HD23	1:22:A:ILE:HD12	8	0.18
(1,78)	1:39:A:LYS:H	1:38:A:GLU:HA	8	0.18
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	8	0.18
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	3	0.18
(1,25)	1:71:A:LEU:H	1:115:A:THR:HG21	3	0.18
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	5	0.18
(3,56)	1:34:A:VAL:N	1:48:A:LYS:O	8	0.17
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	8	0.17
(2,1060)	1:107:A:TYR:HE1	1:3:A:LYS:HE3	8	0.17
(2,1035)	1:32:A:VAL:HG21	1:92:A:MET:HE2	1	0.17
(2,1035)	1:32:A:VAL:HG22	1:92:A:MET:HE2	2	0.17
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	1	0.17
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	2	0.17
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD13	1	0.17
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD13	2	0.17
(2,957)	1:12:A:LEU:HD11	1:12:A:LEU:HD13	3	0.17
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD11	4	0.17
(2,957)	1:12:A:LEU:HD11	1:12:A:LEU:HD13	5	0.17
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD11	6	0.17
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD13	7	0.17
(2,957)	1:12:A:LEU:HD11	1:12:A:LEU:HD13	8	0.17
(2,957)	1:12:A:LEU:HD12	1:12:A:LEU:HD11	9	0.17
(2,957)	1:12:A:LEU:HD11	1:12:A:LEU:HD13	10	0.17
(2,954)	1:12:A:LEU:HD21	1:12:A:LEU:HD11	1	0.17
(2,954)	1:12:A:LEU:HD21	1:12:A:LEU:HD11	8	0.17
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD13	2	0.17
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG2	9	0.17
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	10	0.17
(2,930)	1:3:A:LYS:HE3	1:3:A:LYS:HG3	5	0.17
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD23	2	0.17
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG22	10	0.17
(2,888)	1:92:A:MET:HE2	1:108:A:VAL:HG22	2	0.17
(2,882)	1:45:A:ILE:HG21	1:47:A:LYS:HB3	8	0.17
(2,876)	1:18:A:GLU:HG2	1:22:A:ILE:HD13	5	0.17
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB1	2	0.17
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB2	3	0.17
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB3	7	0.17
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB2	9	0.17
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB2	10	0.17
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB1	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB2	3	0.17
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB2	4	0.17
(2,819)	1:73:A:ALA:HB2	1:74:A:GLU:HB2	3	0.17
(2,819)	1:73:A:ALA:HB3	1:74:A:GLU:HB2	5	0.17
(2,819)	1:73:A:ALA:HB2	1:74:A:GLU:HB2	6	0.17
(2,819)	1:73:A:ALA:HB1	1:74:A:GLU:HB2	8	0.17
(2,808)	1:32:A:VAL:HG21	1:32:A:VAL:HG11	1	0.17
(2,799)	1:108:A:VAL:HG11	1:92:A:MET:HE1	7	0.17
(2,796)	1:32:A:VAL:HG12	1:32:A:VAL:HB	9	0.17
(2,791)	1:95:A:VAL:HG22	1:95:A:VAL:HB	8	0.17
(2,791)	1:95:A:VAL:HG21	1:95:A:VAL:HB	10	0.17
(2,779)	1:109:A:THR:HG21	1:80:A:PHE:HB2	7	0.17
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	3	0.17
(2,756)	1:57:A:THR:HG21	1:57:A:THR:HA	4	0.17
(2,755)	1:109:A:THR:HG22	1:109:A:THR:HA	8	0.17
(2,753)	1:115:A:THR:HG21	1:116:A:PHE:HD1	2	0.17
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD13	10	0.17
(2,712)	1:91:A:LEU:HG	1:91:A:LEU:HA	3	0.17
(2,692)	1:71:A:LEU:HG	1:67:A:LYS:HB2	10	0.17
(2,677)	1:85:A:LEU:HD13	1:78:A:PHE:HD1	4	0.17
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	2	0.17
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	4	0.17
(2,669)	1:70:A:LYS:HD2	1:70:A:LYS:HB3	6	0.17
(2,644)	1:113:A:GLU:H	1:113:A:GLU:HB2	8	0.17
(2,622)	1:75:A:LYS:HB2	1:76:A:ALA:H	3	0.17
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	6	0.17
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	10	0.17
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	2	0.17
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	5	0.17
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	1	0.17
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	2	0.17
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	3	0.17
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	4	0.17
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	7	0.17
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	8	0.17
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	9	0.17
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG22	5	0.17
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG23	9	0.17
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	2	0.17
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	1	0.17
(2,499)	1:116:A:PHE:HA	1:115:A:THR:HG22	8	0.17
(2,490)	1:9:A:GLU:HA	1:9:A:GLU:HG3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,490)	1:9:A:GLU:HA	1:9:A:GLU:HG3	7	0.17
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG13	5	0.17
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG11	7	0.17
(2,449)	1:63:A:TYR:HA	1:67:A:LYS:HD2	6	0.17
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	2	0.17
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	2	0.17
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	3	0.17
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	5	0.17
(2,228)	1:96:A:TYR:H	1:30:A:ILE:HD12	7	0.17
(2,221)	1:49:A:LYS:H	1:49:A:LYS:HD2	4	0.17
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB2	8	0.17
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB1	9	0.17
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	9	0.17
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	9	0.17
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	3	0.17
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	8	0.17
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	4	0.17
(2,26)	1:32:A:VAL:H	1:32:A:VAL:HG12	9	0.17
(1,246)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	7	0.17
(1,246)	1:34:A:VAL:HG13	1:65:A:ILE:HD13	10	0.17
(1,225)	1:32:A:VAL:HG12	1:32:A:VAL:HA	4	0.17
(1,214)	1:35:A:GLU:HG3	1:5:A:SER:HA	7	0.17
(1,195)	1:42:A:ILE:HD11	1:77:A:ILE:HA	3	0.17
(1,182)	1:30:A:ILE:HG22	1:32:A:VAL:HB	1	0.17
(1,182)	1:30:A:ILE:HG22	1:32:A:VAL:HB	3	0.17
(1,178)	1:33:A:ILE:HG21	1:6:A:PHE:HB2	7	0.17
(1,178)	1:33:A:ILE:HG21	1:6:A:PHE:HB2	8	0.17
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB1	9	0.17
(1,172)	1:30:A:ILE:HG23	1:52:A:VAL:H	6	0.17
(1,165)	1:32:A:VAL:HG22	1:32:A:VAL:HG13	7	0.17
(1,160)	1:12:A:LEU:HD13	1:15:A:ARG:HB2	10	0.17
(1,156)	1:34:A:VAL:HG11	1:110:A:TYR:H	1	0.17
(1,150)	1:71:A:LEU:HD13	1:42:A:ILE:HG13	2	0.17
(1,127)	1:3:A:LYS:HB3	1:109:A:THR:HB	1	0.17
(1,127)	1:3:A:LYS:HB3	1:109:A:THR:HB	7	0.17
(1,104)	1:47:A:LYS:HE3	1:5:A:SER:HB2	1	0.17
(1,78)	1:12:A:LEU:HA	1:13:A:GLU:H	2	0.17
(1,68)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	5	0.17
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG22	6	0.17
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	2	0.17
(1,38)	1:113:A:GLU:H	1:113:A:GLU:HB3	7	0.17
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG13	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1062)	1:50:A:TYR:HE1	1:64:A:VAL:HG11	9	0.16
(2,1048)	1:54:A:ALA:HB2	1:30:A:ILE:HD12	5	0.16
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	4	0.16
(2,1017)	1:79:A:ILE:HG23	1:108:A:VAL:HG13	6	0.16
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG21	6	0.16
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG23	1	0.16
(2,983)	1:108:A:VAL:HG21	1:108:A:VAL:HG23	2	0.16
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG23	3	0.16
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG21	4	0.16
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG21	5	0.16
(2,983)	1:108:A:VAL:HG21	1:108:A:VAL:HG23	6	0.16
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG21	7	0.16
(2,983)	1:108:A:VAL:HG21	1:108:A:VAL:HG23	8	0.16
(2,983)	1:108:A:VAL:HG21	1:108:A:VAL:HG23	9	0.16
(2,983)	1:108:A:VAL:HG22	1:108:A:VAL:HG23	10	0.16
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	4	0.16
(2,935)	1:91:A:LEU:HB3	1:91:A:LEU:HD11	8	0.16
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	2	0.16
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	10	0.16
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD13	4	0.16
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB3	2	0.16
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB1	3	0.16
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB3	5	0.16
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB3	6	0.16
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB1	8	0.16
(2,825)	1:34:A:VAL:H	1:33:A:ILE:HG22	4	0.16
(2,819)	1:73:A:ALA:HB3	1:74:A:GLU:HB2	1	0.16
(2,819)	1:73:A:ALA:HB1	1:74:A:GLU:HB2	9	0.16
(2,819)	1:73:A:ALA:HB2	1:74:A:GLU:HB2	10	0.16
(2,808)	1:32:A:VAL:HG22	1:32:A:VAL:HG13	6	0.16
(2,796)	1:32:A:VAL:HG12	1:32:A:VAL:HB	1	0.16
(2,796)	1:32:A:VAL:HG11	1:32:A:VAL:HB	3	0.16
(2,791)	1:95:A:VAL:HG21	1:95:A:VAL:HB	4	0.16
(2,784)	1:57:A:THR:HG22	1:60:A:GLN:HB2	9	0.16
(2,779)	1:109:A:THR:HG23	1:80:A:PHE:HB2	8	0.16
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG22	4	0.16
(2,770)	1:115:A:THR:HG21	1:115:A:THR:HA	9	0.16
(2,762)	1:57:A:THR:HG23	1:56:A:LEU:HA	4	0.16
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD11	2	0.16
(2,622)	1:75:A:LYS:HB2	1:76:A:ALA:H	6	0.16
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	5	0.16
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,579)	1:22:A:ILE:H	1:22:A:ILE:HB	10	0.16
(2,552)	1:16:A:ARG:HD2	1:20:A:ALA:HB2	10	0.16
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	6	0.16
(2,542)	1:70:A:LYS:HE2	1:44:A:THR:HB	9	0.16
(2,455)	1:96:A:TYR:HA	1:95:A:VAL:HG13	4	0.16
(2,401)	1:71:A:LEU:HG	1:69:A:ILE:HD13	3	0.16
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	6	0.16
(2,362)	1:93:A:SER:H	1:95:A:VAL:HB	3	0.16
(2,350)	1:99:A:LYS:H	1:95:A:VAL:HG13	7	0.16
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	7	0.16
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	8	0.16
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	5	0.16
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	7	0.16
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB2	5	0.16
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB1	10	0.16
(2,219)	1:49:A:LYS:H	1:48:A:LYS:HB3	4	0.16
(2,209)	1:118:A:PHE:H	1:118:A:PHE:HB3	9	0.16
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	7	0.16
(2,76)	1:101:A:ASP:H	1:100:A:LYS:HG3	5	0.16
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD1	1	0.16
(1,244)	1:42:A:ILE:HD11	1:69:A:ILE:HD13	1	0.16
(1,244)	1:42:A:ILE:HD13	1:69:A:ILE:HD12	6	0.16
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB1	7	0.16
(1,172)	1:30:A:ILE:HG22	1:52:A:VAL:H	3	0.16
(1,127)	1:3:A:LYS:HB2	1:109:A:THR:HB	4	0.16
(1,103)	1:16:A:ARG:HD3	1:103:A:ASP:HA	1	0.16
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	1	0.16
(1,68)	1:62:A:VAL:HG11	1:77:A:ILE:HG22	7	0.16
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	9	0.16
(1,54)	1:111:A:SER:H	1:110:A:TYR:HB3	4	0.16
(1,49)	1:67:A:LYS:H	1:65:A:ILE:H	1	0.16
(1,49)	1:67:A:LYS:H	1:65:A:ILE:H	6	0.16
(1,48)	1:79:A:ILE:H	1:80:A:PHE:H	10	0.16
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG12	8	0.16
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	8	0.16
(3,56)	1:34:A:VAL:N	1:48:A:LYS:O	4	0.15
(3,51)	1:33:A:ILE:N	1:106:A:LEU:O	5	0.15
(3,49)	1:37:A:ALA:N	1:110:A:TYR:O	6	0.15
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	3	0.15
(3,43)	1:97:A:GLU:N	1:93:A:SER:O	10	0.15
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	3	0.15
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1054)	1:107:A:TYR:HD1	1:107:A:TYR:HB2	5	0.15
(2,1050)	1:30:A:ILE:HD11	1:30:A:ILE:HD13	1	0.15
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD13	2	0.15
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD13	5	0.15
(2,1050)	1:30:A:ILE:HD11	1:30:A:ILE:HD13	8	0.15
(2,1050)	1:30:A:ILE:HD11	1:30:A:ILE:HD13	10	0.15
(2,1048)	1:54:A:ALA:HB3	1:30:A:ILE:HD12	1	0.15
(2,1048)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	3	0.15
(2,1036)	1:30:A:ILE:HG23	1:92:A:MET:HE1	2	0.15
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	5	0.15
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG13	7	0.15
(2,1017)	1:79:A:ILE:HG21	1:108:A:VAL:HG11	8	0.15
(2,978)	1:81:A:VAL:HG11	1:3:A:LYS:HG2	8	0.15
(2,967)	1:32:A:VAL:HG23	1:108:A:VAL:HG21	3	0.15
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	5	0.15
(2,954)	1:12:A:LEU:HD23	1:12:A:LEU:HD11	10	0.15
(2,944)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	10	0.15
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG3	8	0.15
(2,932)	1:113:A:GLU:HG3	1:75:A:LYS:HG3	9	0.15
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD21	8	0.15
(2,908)	1:77:A:ILE:HD12	1:79:A:ILE:HD12	10	0.15
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG22	7	0.15
(2,869)	1:92:A:MET:HE1	1:58:A:VAL:HA	4	0.15
(2,867)	1:92:A:MET:HE1	1:61:A:PHE:HD2	8	0.15
(2,867)	1:92:A:MET:HE1	1:61:A:PHE:HD2	9	0.15
(2,862)	1:112:A:GLY:H	1:42:A:ILE:HD11	3	0.15
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB2	5	0.15
(2,800)	1:95:A:VAL:HG22	1:90:A:ALA:HB2	6	0.15
(2,791)	1:95:A:VAL:HG21	1:95:A:VAL:HB	5	0.15
(2,784)	1:57:A:THR:HG23	1:60:A:GLN:HB2	2	0.15
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG22	1	0.15
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG23	3	0.15
(2,720)	1:78:A:PHE:HB3	1:85:A:LEU:HD22	1	0.15
(2,718)	1:3:A:LYS:HE2	1:3:A:LYS:HG2	7	0.15
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD13	8	0.15
(2,677)	1:85:A:LEU:HD11	1:78:A:PHE:HD2	1	0.15
(2,677)	1:85:A:LEU:HD12	1:78:A:PHE:HD2	7	0.15
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	10	0.15
(2,622)	1:75:A:LYS:HB2	1:76:A:ALA:H	4	0.15
(2,565)	1:39:A:LYS:HE3	1:38:A:GLU:H	6	0.15
(2,555)	1:70:A:LYS:HE3	1:42:A:ILE:HG12	4	0.15
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	5	0.15
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	3	0.15
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG21	7	0.15
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG21	9	0.15
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG21	10	0.15
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	5	0.15
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB1	9	0.15
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	10	0.15
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	6	0.15
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	8	0.15
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	2	0.15
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	7	0.15
(2,220)	1:21:A:ARG:H	1:20:A:ALA:HB2	7	0.15
(2,205)	1:62:A:VAL:H	1:59:A:GLY:HA3	1	0.15
(2,139)	1:116:A:PHE:H	1:116:A:PHE:HB3	10	0.15
(2,138)	1:116:A:PHE:H	1:116:A:PHE:HB2	6	0.15
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	3	0.15
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	2	0.15
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	4	0.15
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	6	0.15
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD1	7	0.15
(2,26)	1:32:A:VAL:H	1:32:A:VAL:HG12	1	0.15
(1,244)	1:42:A:ILE:HD13	1:69:A:ILE:HD13	3	0.15
(1,244)	1:42:A:ILE:HD11	1:69:A:ILE:HD13	7	0.15
(1,230)	1:109:A:THR:HG22	1:109:A:THR:HA	4	0.15
(1,230)	1:109:A:THR:HG22	1:109:A:THR:HA	6	0.15
(1,225)	1:32:A:VAL:HG12	1:32:A:VAL:HA	5	0.15
(1,182)	1:30:A:ILE:HG23	1:32:A:VAL:HB	4	0.15
(1,174)	1:33:A:ILE:HG23	1:107:A:TYR:HE2	5	0.15
(1,150)	1:71:A:LEU:HD11	1:42:A:ILE:HG13	7	0.15
(1,150)	1:71:A:LEU:HD12	1:42:A:ILE:HG13	8	0.15
(1,128)	1:3:A:LYS:HB3	1:35:A:GLU:HB2	6	0.15
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	10	0.15
(1,101)	1:106:A:LEU:HB3	1:31:A:PRO:HB2	9	0.15
(1,68)	1:62:A:VAL:HG12	1:77:A:ILE:HG22	4	0.15
(1,49)	1:67:A:LYS:H	1:65:A:ILE:H	3	0.15
(1,48)	1:79:A:ILE:H	1:80:A:PHE:H	9	0.15
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	6	0.15
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG13	4	0.15
(3,56)	1:34:A:VAL:N	1:48:A:LYS:O	2	0.14
(3,41)	1:98:A:GLU:N	1:94:A:SER:O	2	0.14
(3,23)	1:15:A:ARG:N	1:11:A:ASP:O	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:16:A:ARG:N	1:12:A:LEU:O	1	0.14
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	4	0.14
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	2	0.14
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	6	0.14
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	7	0.14
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	8	0.14
(2,1062)	1:50:A:TYR:HE1	1:64:A:VAL:HG13	10	0.14
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD13	3	0.14
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD13	4	0.14
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD11	6	0.14
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD13	7	0.14
(2,1050)	1:30:A:ILE:HD12	1:30:A:ILE:HD13	9	0.14
(2,1048)	1:54:A:ALA:HB1	1:30:A:ILE:HD12	9	0.14
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG21	10	0.14
(2,978)	1:81:A:VAL:HG12	1:3:A:LYS:HG2	6	0.14
(2,962)	1:34:A:VAL:HG12	1:45:A:ILE:HG12	10	0.14
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG21	1	0.14
(2,905)	1:79:A:ILE:HD13	1:62:A:VAL:HG22	6	0.14
(2,901)	1:79:A:ILE:HD13	1:79:A:ILE:HB	1	0.14
(2,899)	1:65:A:ILE:HD12	1:61:A:PHE:HE1	9	0.14
(2,892)	1:69:A:ILE:HG23	1:69:A:ILE:HD11	10	0.14
(2,870)	1:42:A:ILE:HD11	1:67:A:LYS:HA	1	0.14
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB1	7	0.14
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB3	9	0.14
(2,835)	1:17:A:ALA:HA	1:17:A:ALA:HB3	10	0.14
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB1	7	0.14
(2,819)	1:73:A:ALA:HB1	1:74:A:GLU:HB2	2	0.14
(2,819)	1:73:A:ALA:HB1	1:74:A:GLU:HB2	4	0.14
(2,808)	1:32:A:VAL:HG23	1:32:A:VAL:HG13	3	0.14
(2,780)	1:115:A:THR:HG22	1:116:A:PHE:HB3	8	0.14
(2,779)	1:109:A:THR:HG23	1:80:A:PHE:HB2	3	0.14
(2,779)	1:109:A:THR:HG21	1:80:A:PHE:HB2	10	0.14
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG23	8	0.14
(2,726)	1:67:A:LYS:HG2	1:67:A:LYS:HD3	8	0.14
(2,725)	1:91:A:LEU:HG	1:91:A:LEU:HB3	3	0.14
(2,708)	1:85:A:LEU:HD21	1:80:A:PHE:HA	5	0.14
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD23	9	0.14
(2,677)	1:85:A:LEU:HD13	1:78:A:PHE:HD1	2	0.14
(2,677)	1:85:A:LEU:HD11	1:78:A:PHE:HD2	8	0.14
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG2	1	0.14
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	8	0.14
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,610)	1:13:A:GLU:HA	1:13:A:GLU:HG2	4	0.14
(2,607)	1:113:A:GLU:HG3	1:113:A:GLU:HA	8	0.14
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG21	7	0.14
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	2	0.14
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	4	0.14
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	5	0.14
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	6	0.14
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	7	0.14
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	9	0.14
(2,565)	1:39:A:LYS:HE3	1:38:A:GLU:H	3	0.14
(2,559)	1:3:A:LYS:HE3	1:81:A:VAL:HG11	5	0.14
(2,555)	1:70:A:LYS:HE3	1:42:A:ILE:HG13	9	0.14
(2,547)	1:70:A:LYS:HE3	1:43:A:PRO:HG2	6	0.14
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	10	0.14
(2,544)	1:47:A:LYS:HE3	1:48:A:LYS:HA	2	0.14
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG22	2	0.14
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG22	6	0.14
(2,463)	1:60:A:GLN:HA	1:60:A:GLN:HG2	8	0.14
(2,440)	1:6:A:PHE:HA	1:6:A:PHE:HD1	2	0.14
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	9	0.14
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB1	10	0.14
(2,346)	1:99:A:LYS:H	1:98:A:GLU:HB2	6	0.14
(2,343)	1:99:A:LYS:H	1:100:A:LYS:HA	4	0.14
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	1	0.14
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	8	0.14
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD3	1	0.14
(2,209)	1:118:A:PHE:H	1:118:A:PHE:HB3	3	0.14
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	10	0.14
(2,182)	1:60:A:GLN:H	1:57:A:THR:HG23	4	0.14
(2,181)	1:100:A:LYS:H	1:100:A:LYS:HG2	6	0.14
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	5	0.14
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	8	0.14
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	9	0.14
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	1	0.14
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	10	0.14
(2,26)	1:32:A:VAL:H	1:32:A:VAL:HG13	2	0.14
(2,10)	1:85:A:LEU:H	1:80:A:PHE:HD2	6	0.14
(1,248)	1:50:A:TYR:HE1	1:52:A:VAL:HB	7	0.14
(1,246)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	9	0.14
(1,242)	1:65:A:ILE:HG22	1:77:A:ILE:HD13	10	0.14
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG22	10	0.14
(1,212)	1:33:A:ILE:HD13	1:49:A:LYS:HG3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:22:A:ILE:HD13	1:51:A:LEU:HD13	3	0.14
(1,201)	1:22:A:ILE:HD12	1:51:A:LEU:HD13	9	0.14
(1,188)	1:54:A:ALA:HB2	1:30:A:ILE:HG13	5	0.14
(1,187)	1:58:A:VAL:HG22	1:90:A:ALA:HB2	6	0.14
(1,182)	1:30:A:ILE:HG23	1:32:A:VAL:HB	6	0.14
(1,169)	1:54:A:ALA:HB1	1:30:A:ILE:HD13	10	0.14
(1,152)	1:109:A:THR:HG23	1:80:A:PHE:H	4	0.14
(1,128)	1:3:A:LYS:HB3	1:35:A:GLU:HB2	2	0.14
(1,105)	1:67:A:LYS:HE3	1:63:A:TYR:HA	2	0.14
(1,78)	1:39:A:LYS:H	1:38:A:GLU:HA	4	0.14
(1,78)	1:39:A:LYS:H	1:38:A:GLU:HA	5	0.14
(1,68)	1:62:A:VAL:HG13	1:77:A:ILE:HG23	2	0.14
(1,55)	1:111:A:SER:H	1:42:A:ILE:HG21	3	0.14
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	4	0.14
(3,56)	1:34:A:VAL:N	1:48:A:LYS:O	3	0.13
(3,49)	1:37:A:ALA:N	1:110:A:TYR:O	8	0.13
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	2	0.13
(3,43)	1:97:A:GLU:N	1:93:A:SER:O	4	0.13
(2,1054)	1:107:A:TYR:HD1	1:107:A:TYR:HB2	4	0.13
(2,954)	1:12:A:LEU:HD21	1:12:A:LEU:HD13	4	0.13
(2,954)	1:12:A:LEU:HD21	1:12:A:LEU:HD11	5	0.13
(2,944)	1:71:A:LEU:HD22	1:71:A:LEU:HB2	5	0.13
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG2	4	0.13
(2,933)	1:39:A:LYS:HG3	1:38:A:GLU:HG2	5	0.13
(2,931)	1:48:A:LYS:HG2	1:47:A:LYS:HE2	3	0.13
(2,905)	1:79:A:ILE:HD12	1:62:A:VAL:HG21	2	0.13
(2,901)	1:79:A:ILE:HD13	1:79:A:ILE:HB	4	0.13
(2,901)	1:79:A:ILE:HD13	1:79:A:ILE:HB	10	0.13
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB1	5	0.13
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB1	6	0.13
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB3	10	0.13
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB2	6	0.13
(2,821)	1:76:A:ALA:HB3	1:67:A:LYS:HB3	2	0.13
(2,800)	1:95:A:VAL:HG22	1:90:A:ALA:HB1	3	0.13
(2,798)	1:109:A:THR:HG23	1:37:A:ALA:HB3	5	0.13
(2,784)	1:57:A:THR:HG23	1:60:A:GLN:HB2	6	0.13
(2,777)	1:12:A:LEU:HD11	1:103:A:ASP:HB2	1	0.13
(2,770)	1:115:A:THR:HG22	1:115:A:THR:HA	7	0.13
(2,755)	1:109:A:THR:HG23	1:109:A:THR:HA	7	0.13
(2,754)	1:34:A:VAL:HG22	1:50:A:TYR:HE2	1	0.13
(2,685)	1:96:A:TYR:HA	1:106:A:LEU:HD21	2	0.13
(2,677)	1:85:A:LEU:HD12	1:78:A:PHE:HD1	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG2	7	0.13
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	3	0.13
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	5	0.13
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	6	0.13
(2,622)	1:75:A:LYS:HB2	1:76:A:ALA:H	8	0.13
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	1	0.13
(2,614)	1:98:A:GLU:HG3	1:97:A:GLU:HG3	7	0.13
(2,610)	1:13:A:GLU:HA	1:13:A:GLU:HG2	8	0.13
(2,566)	1:41:A:ASP:HB2	1:41:A:ASP:HA	3	0.13
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	7	0.13
(2,555)	1:70:A:LYS:HE3	1:42:A:ILE:HG12	5	0.13
(2,490)	1:9:A:GLU:HA	1:9:A:GLU:HG3	8	0.13
(2,484)	1:3:A:LYS:HA	1:109:A:THR:HB	3	0.13
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	2	0.13
(2,463)	1:60:A:GLN:HA	1:60:A:GLN:HG2	5	0.13
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	10	0.13
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	2	0.13
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	3	0.13
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB3	1	0.13
(2,366)	1:93:A:SER:H	1:54:A:ALA:HB3	6	0.13
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	4	0.13
(2,341)	1:77:A:ILE:H	1:76:A:ALA:HA	5	0.13
(2,259)	1:16:A:ARG:H	1:16:A:ARG:HD3	4	0.13
(2,253)	1:113:A:GLU:H	1:115:A:THR:HB	8	0.13
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	6	0.13
(2,226)	1:65:A:ILE:H	1:65:A:ILE:HG12	10	0.13
(2,221)	1:49:A:LYS:H	1:49:A:LYS:HD2	2	0.13
(2,221)	1:49:A:LYS:H	1:49:A:LYS:HD2	6	0.13
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	1	0.13
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	3	0.13
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	6	0.13
(2,131)	1:75:A:LYS:H	1:74:A:GLU:HA	4	0.13
(2,131)	1:75:A:LYS:H	1:74:A:GLU:HA	5	0.13
(2,131)	1:75:A:LYS:H	1:74:A:GLU:HA	10	0.13
(2,121)	1:14:A:LYS:H	1:13:A:GLU:H	5	0.13
(2,98)	1:19:A:ALA:H	1:17:A:ALA:HA	7	0.13
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD1	8	0.13
(2,10)	1:85:A:LEU:H	1:80:A:PHE:HD2	1	0.13
(2,10)	1:85:A:LEU:H	1:80:A:PHE:HD1	5	0.13
(1,248)	1:50:A:TYR:HE1	1:52:A:VAL:HB	10	0.13
(1,244)	1:42:A:ILE:HD11	1:69:A:ILE:HD13	2	0.13
(1,244)	1:42:A:ILE:HD12	1:69:A:ILE:HD13	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:42:A:ILE:HD13	1:69:A:ILE:HD12	8	0.13
(1,232)	1:3:A:LYS:HG2	1:109:A:THR:HG21	5	0.13
(1,133)	1:75:A:LYS:HB3	1:71:A:LEU:HD11	1	0.13
(1,130)	1:3:A:LYS:HB2	1:3:A:LYS:HG3	9	0.13
(1,127)	1:3:A:LYS:HB3	1:109:A:THR:HB	6	0.13
(1,127)	1:3:A:LYS:HB3	1:109:A:THR:HB	9	0.13
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	9	0.13
(1,99)	1:53:A:PRO:HD3	1:29:A:ARG:HB2	4	0.13
(1,91)	1:88:A:ALA:HA	1:62:A:VAL:HG23	2	0.13
(1,91)	1:88:A:ALA:HA	1:62:A:VAL:HG22	9	0.13
(1,49)	1:67:A:LYS:H	1:65:A:ILE:H	8	0.13
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG21	8	0.13
(1,38)	1:113:A:GLU:H	1:113:A:GLU:HB3	4	0.13
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG12	3	0.13
(3,56)	1:34:A:VAL:N	1:48:A:LYS:O	5	0.12
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	1	0.12
(3,43)	1:97:A:GLU:N	1:93:A:SER:O	5	0.12
(3,42)	1:98:A:GLU:H	1:94:A:SER:O	6	0.12
(3,42)	1:98:A:GLU:H	1:94:A:SER:O	10	0.12
(3,20)	1:17:A:ALA:H	1:13:A:GLU:O	2	0.12
(3,20)	1:17:A:ALA:H	1:13:A:GLU:O	4	0.12
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	3	0.12
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	5	0.12
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	6	0.12
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	9	0.12
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	1	0.12
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	5	0.12
(2,1062)	1:50:A:TYR:HE1	1:64:A:VAL:HG12	1	0.12
(2,1060)	1:107:A:TYR:HE1	1:3:A:LYS:HE2	10	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG21	1	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG21	2	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG21	3	0.12
(2,1009)	1:42:A:ILE:HG21	1:42:A:ILE:HG23	4	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG21	5	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG23	6	0.12
(2,1009)	1:42:A:ILE:HG21	1:42:A:ILE:HG23	7	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG21	8	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG23	9	0.12
(2,1009)	1:42:A:ILE:HG22	1:42:A:ILE:HG21	10	0.12
(2,974)	1:115:A:THR:HG21	1:116:A:PHE:HB2	2	0.12
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD21	7	0.12
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD21	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,901)	1:79:A:ILE:HD13	1:79:A:ILE:HB	2	0.12
(2,859)	1:30:A:ILE:HG23	1:30:A:ILE:HG13	5	0.12
(2,839)	1:20:A:ALA:HA	1:20:A:ALA:HB1	8	0.12
(2,798)	1:109:A:THR:HG22	1:37:A:ALA:HB2	9	0.12
(2,791)	1:95:A:VAL:HG22	1:95:A:VAL:HB	2	0.12
(2,780)	1:115:A:THR:HG23	1:116:A:PHE:HB3	7	0.12
(2,772)	1:115:A:THR:HB	1:115:A:THR:HG21	2	0.12
(2,768)	1:12:A:LEU:HA	1:12:A:LEU:HD13	2	0.12
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG23	2	0.12
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG22	3	0.12
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD22	7	0.12
(2,730)	1:71:A:LEU:HD11	1:67:A:LYS:HB3	8	0.12
(2,713)	1:71:A:LEU:HA	1:71:A:LEU:HD11	5	0.12
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	3	0.12
(2,669)	1:70:A:LYS:HD3	1:70:A:LYS:HB2	7	0.12
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	1	0.12
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	9	0.12
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	8	0.12
(2,614)	1:98:A:GLU:HG3	1:97:A:GLU:HG3	8	0.12
(2,604)	1:85:A:LEU:H	1:84:A:VAL:HB	2	0.12
(2,576)	1:45:A:ILE:HB	1:44:A:THR:HG21	1	0.12
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	1	0.12
(2,560)	1:110:A:TYR:HB2	1:34:A:VAL:HG13	5	0.12
(2,555)	1:70:A:LYS:HE3	1:42:A:ILE:HG12	1	0.12
(2,554)	1:39:A:LYS:HE2	1:39:A:LYS:HD3	8	0.12
(2,490)	1:9:A:GLU:HA	1:9:A:GLU:HG3	5	0.12
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG23	3	0.12
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	5	0.12
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	10	0.12
(2,463)	1:60:A:GLN:HA	1:60:A:GLN:HG2	9	0.12
(2,450)	1:44:A:THR:HA	1:44:A:THR:HG23	4	0.12
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	5	0.12
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	6	0.12
(2,410)	1:58:A:VAL:HA	1:61:A:PHE:HB2	2	0.12
(2,375)	1:69:A:ILE:H	1:71:A:LEU:HG	9	0.12
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	1	0.12
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	2	0.12
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	8	0.12
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	9	0.12
(2,346)	1:99:A:LYS:H	1:98:A:GLU:HB2	9	0.12
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	4	0.12
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	3	0.12
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	4	0.12
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	6	0.12
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	9	0.12
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	10	0.12
(2,261)	1:66:A:ARG:H	1:62:A:VAL:HA	1	0.12
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	9	0.12
(2,219)	1:49:A:LYS:H	1:48:A:LYS:HB3	5	0.12
(2,205)	1:62:A:VAL:H	1:59:A:GLY:HA3	2	0.12
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	1	0.12
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	2	0.12
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	3	0.12
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	4	0.12
(2,176)	1:17:A:ALA:H	1:16:A:ARG:HB3	9	0.12
(2,139)	1:116:A:PHE:H	1:116:A:PHE:HB3	5	0.12
(2,136)	1:71:A:LEU:H	1:70:A:LYS:HA	6	0.12
(2,135)	1:75:A:LYS:H	1:73:A:ALA:HA	4	0.12
(2,70)	1:78:A:PHE:H	1:78:A:PHE:HB3	9	0.12
(2,55)	1:61:A:PHE:H	1:61:A:PHE:HD2	7	0.12
(2,50)	1:108:A:VAL:H	1:109:A:THR:H	4	0.12
(1,244)	1:42:A:ILE:HD12	1:69:A:ILE:HD13	5	0.12
(1,244)	1:42:A:ILE:HD12	1:69:A:ILE:HD13	10	0.12
(1,240)	1:69:A:ILE:HG23	1:69:A:ILE:HD11	2	0.12
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG21	9	0.12
(1,214)	1:35:A:GLU:HG2	1:5:A:SER:HA	8	0.12
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB1	3	0.12
(1,175)	1:111:A:SER:HB3	1:37:A:ALA:HB2	8	0.12
(1,162)	1:32:A:VAL:HG22	1:106:A:LEU:HB3	3	0.12
(1,156)	1:34:A:VAL:HG13	1:110:A:TYR:H	2	0.12
(1,154)	1:110:A:TYR:H	1:109:A:THR:HG23	10	0.12
(1,153)	1:32:A:VAL:H	1:52:A:VAL:HG23	9	0.12
(1,150)	1:71:A:LEU:HD13	1:42:A:ILE:HG13	6	0.12
(1,130)	1:3:A:LYS:HB2	1:3:A:LYS:HG2	6	0.12
(1,127)	1:3:A:LYS:HB3	1:109:A:THR:HB	3	0.12
(1,127)	1:3:A:LYS:HB2	1:109:A:THR:HB	10	0.12
(1,104)	1:47:A:LYS:HE3	1:5:A:SER:HB2	3	0.12
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	1	0.12
(1,78)	1:12:A:LEU:HA	1:13:A:GLU:H	3	0.12
(1,78)	1:12:A:LEU:HA	1:13:A:GLU:H	9	0.12
(1,48)	1:79:A:ILE:H	1:80:A:PHE:H	4	0.12
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG21	3	0.12
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG23	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG21	6	0.12
(1,9)	1:108:A:VAL:H	1:107:A:TYR:HD1	1	0.12
(1,7)	1:45:A:ILE:H	1:44:A:THR:HA	6	0.12
(3,51)	1:33:A:ILE:N	1:106:A:LEU:O	8	0.11
(3,51)	1:33:A:ILE:N	1:106:A:LEU:O	9	0.11
(3,50)	1:35:A:GLU:N	1:108:A:VAL:O	8	0.11
(3,44)	1:97:A:GLU:H	1:93:A:SER:O	9	0.11
(3,43)	1:97:A:GLU:N	1:93:A:SER:O	8	0.11
(3,42)	1:98:A:GLU:H	1:94:A:SER:O	8	0.11
(3,21)	1:16:A:ARG:N	1:12:A:LEU:O	4	0.11
(3,19)	1:17:A:ALA:N	1:13:A:GLU:O	2	0.11
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	2	0.11
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	8	0.11
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	2	0.11
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	7	0.11
(3,7)	1:23:A:ARG:N	1:19:A:ALA:O	10	0.11
(3,6)	1:24:A:GLU:H	1:20:A:ALA:O	7	0.11
(3,6)	1:24:A:GLU:H	1:20:A:ALA:O	8	0.11
(3,1)	1:26:A:TYR:N	1:22:A:ILE:O	3	0.11
(3,1)	1:26:A:TYR:N	1:22:A:ILE:O	9	0.11
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG22	1	0.11
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG22	4	0.11
(2,973)	1:70:A:LYS:HE2	1:115:A:THR:HG22	10	0.11
(2,956)	1:100:A:LYS:HG2	1:99:A:LYS:HG3	8	0.11
(2,944)	1:71:A:LEU:HD21	1:71:A:LEU:HB2	7	0.11
(2,930)	1:3:A:LYS:HE3	1:3:A:LYS:HG3	3	0.11
(2,919)	1:57:A:THR:HA	1:91:A:LEU:HD22	4	0.11
(2,901)	1:79:A:ILE:HD12	1:79:A:ILE:HB	8	0.11
(2,882)	1:45:A:ILE:HG23	1:47:A:LYS:HB3	2	0.11
(2,869)	1:92:A:MET:HE1	1:58:A:VAL:HA	8	0.11
(2,867)	1:92:A:MET:HE3	1:61:A:PHE:HD2	7	0.11
(2,829)	1:17:A:ALA:H	1:17:A:ALA:HB3	2	0.11
(2,808)	1:32:A:VAL:HG22	1:32:A:VAL:HG12	2	0.11
(2,791)	1:95:A:VAL:HG23	1:95:A:VAL:HB	1	0.11
(2,791)	1:95:A:VAL:HG23	1:95:A:VAL:HB	3	0.11
(2,791)	1:95:A:VAL:HG22	1:95:A:VAL:HB	9	0.11
(2,784)	1:57:A:THR:HG23	1:60:A:GLN:HB2	1	0.11
(2,783)	1:109:A:THR:HG22	1:35:A:GLU:HB3	4	0.11
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG21	1	0.11
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG22	6	0.11
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG22	7	0.11
(2,763)	1:44:A:THR:HB	1:44:A:THR:HG23	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,749)	1:64:A:VAL:H	1:64:A:VAL:HG22	1	0.11
(2,736)	1:99:A:LYS:HG2	1:95:A:VAL:HG21	3	0.11
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD21	5	0.11
(2,731)	1:85:A:LEU:HB2	1:85:A:LEU:HD21	6	0.11
(2,730)	1:71:A:LEU:HD12	1:67:A:LYS:HB3	6	0.11
(2,720)	1:78:A:PHE:HB3	1:85:A:LEU:HD21	7	0.11
(2,708)	1:85:A:LEU:HD22	1:80:A:PHE:HA	7	0.11
(2,692)	1:71:A:LEU:HG	1:67:A:LYS:HB2	5	0.11
(2,677)	1:85:A:LEU:HD11	1:78:A:PHE:HD2	10	0.11
(2,670)	1:39:A:LYS:HD3	1:39:A:LYS:HB2	10	0.11
(2,663)	1:21:A:ARG:HB3	1:22:A:ILE:H	1	0.11
(2,663)	1:21:A:ARG:HB3	1:22:A:ILE:H	4	0.11
(2,663)	1:21:A:ARG:HB3	1:22:A:ILE:H	9	0.11
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	2	0.11
(2,638)	1:25:A:LYS:HB2	1:21:A:ARG:HG3	7	0.11
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	3	0.11
(2,621)	1:81:A:VAL:H	1:81:A:VAL:HB	4	0.11
(2,616)	1:24:A:GLU:HG3	1:23:A:ARG:HG2	4	0.11
(2,567)	1:41:A:ASP:HB3	1:41:A:ASP:HA	8	0.11
(2,567)	1:41:A:ASP:HB3	1:41:A:ASP:HA	10	0.11
(2,565)	1:39:A:LYS:HE2	1:38:A:GLU:H	8	0.11
(2,546)	1:16:A:ARG:HD2	1:16:A:ARG:HB3	9	0.11
(2,484)	1:3:A:LYS:HA	1:109:A:THR:HB	2	0.11
(2,483)	1:116:A:PHE:HA	1:116:A:PHE:HD1	3	0.11
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	1	0.11
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	4	0.11
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	7	0.11
(2,467)	1:13:A:GLU:HA	1:13:A:GLU:HB3	9	0.11
(2,463)	1:60:A:GLN:HA	1:60:A:GLN:HG2	7	0.11
(2,443)	1:87:A:PRO:HA	1:87:A:PRO:HB2	1	0.11
(2,443)	1:87:A:PRO:HA	1:87:A:PRO:HB2	2	0.11
(2,443)	1:87:A:PRO:HA	1:87:A:PRO:HB2	9	0.11
(2,406)	1:45:A:ILE:H	1:44:A:THR:HB	9	0.11
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	1	0.11
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	7	0.11
(2,364)	1:93:A:SER:H	1:91:A:LEU:HB3	10	0.11
(2,341)	1:77:A:ILE:H	1:76:A:ALA:HA	4	0.11
(2,341)	1:77:A:ILE:H	1:76:A:ALA:HA	10	0.11
(2,330)	1:8:A:GLN:H	1:9:A:GLU:HB3	4	0.11
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	2	0.11
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	10	0.11
(2,310)	1:10:A:HIS:H	1:9:A:GLU:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,310)	1:10:A:HIS:H	1:9:A:GLU:HB2	6	0.11
(2,283)	1:24:A:GLU:H	1:26:A:TYR:H	5	0.11
(2,276)	1:70:A:LYS:H	1:44:A:THR:HG22	7	0.11
(2,261)	1:66:A:ARG:H	1:62:A:VAL:HA	4	0.11
(2,237)	1:80:A:PHE:H	1:80:A:PHE:HD1	7	0.11
(2,221)	1:49:A:LYS:H	1:49:A:LYS:HD2	1	0.11
(2,207)	1:21:A:ARG:H	1:19:A:ALA:HA	1	0.11
(2,205)	1:62:A:VAL:H	1:59:A:GLY:HA3	6	0.11
(2,192)	1:52:A:VAL:H	1:30:A:ILE:H	8	0.11
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	4	0.11
(2,183)	1:68:A:ARG:H	1:67:A:LYS:HG2	5	0.11
(2,177)	1:64:A:VAL:H	1:62:A:VAL:HB	10	0.11
(2,176)	1:17:A:ALA:H	1:16:A:ARG:HB3	5	0.11
(2,176)	1:17:A:ALA:H	1:16:A:ARG:HB3	8	0.11
(2,121)	1:14:A:LYS:H	1:13:A:GLU:H	1	0.11
(2,121)	1:14:A:LYS:H	1:13:A:GLU:H	2	0.11
(2,119)	1:109:A:THR:H	1:110:A:TYR:H	10	0.11
(2,102)	1:11:A:ASP:H	1:12:A:LEU:HA	3	0.11
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD2	4	0.11
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD2	5	0.11
(2,50)	1:108:A:VAL:H	1:109:A:THR:H	1	0.11
(2,50)	1:108:A:VAL:H	1:109:A:THR:H	7	0.11
(2,9)	1:85:A:LEU:H	1:84:A:VAL:H	2	0.11
(2,3)	1:37:A:ALA:H	1:36:A:LYS:HB2	7	0.11
(1,250)	1:107:A:TYR:HE2	1:6:A:PHE:HB3	10	0.11
(1,246)	1:34:A:VAL:HG13	1:65:A:ILE:HD12	5	0.11
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG23	1	0.11
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG23	2	0.11
(1,239)	1:69:A:ILE:HG21	1:69:A:ILE:HG23	3	0.11
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG23	4	0.11
(1,239)	1:69:A:ILE:HG21	1:69:A:ILE:HG23	5	0.11
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG23	6	0.11
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG23	7	0.11
(1,239)	1:69:A:ILE:HG21	1:69:A:ILE:HG23	8	0.11
(1,239)	1:69:A:ILE:HG22	1:69:A:ILE:HG23	10	0.11
(1,201)	1:22:A:ILE:HD11	1:51:A:LEU:HD13	1	0.11
(1,195)	1:42:A:ILE:HD13	1:77:A:ILE:HA	4	0.11
(1,194)	1:22:A:ILE:HD12	1:105:A:PHE:HE2	8	0.11
(1,187)	1:58:A:VAL:HG21	1:90:A:ALA:HB2	2	0.11
(1,178)	1:33:A:ILE:HG21	1:6:A:PHE:HB2	5	0.11
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	8	0.11
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	10	0.11
(1,78)	1:39:A:LYS:H	1:38:A:GLU:HA	6	0.11
(1,48)	1:79:A:ILE:H	1:80:A:PHE:H	3	0.11
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG23	1	0.11
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG22	9	0.11
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	2	0.11
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	5	0.11
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG11	1	0.11
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG11	7	0.11
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG12	9	0.11
(1,33)	1:103:A:ASP:H	1:102:A:ASP:HB2	1	0.11
(1,19)	1:95:A:VAL:H	1:91:A:LEU:HG	7	0.11
(1,7)	1:45:A:ILE:H	1:44:A:THR:HA	4	0.11
(1,7)	1:45:A:ILE:H	1:44:A:THR:HA	5	0.11
(1,3)	1:76:A:ALA:H	1:78:A:PHE:HE1	1	0.11
(1,3)	1:76:A:ALA:H	1:78:A:PHE:HE2	6	0.11
(3,49)	1:37:A:ALA:N	1:110:A:TYR:O	3	0.1
(3,43)	1:97:A:GLU:N	1:93:A:SER:O	7	0.1
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	4	0.1
(3,11)	1:21:A:ARG:N	1:17:A:ALA:O	7	0.1
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	5	0.1
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	6	0.1
(3,8)	1:23:A:ARG:H	1:19:A:ALA:O	9	0.1
(3,1)	1:26:A:TYR:N	1:22:A:ILE:O	1	0.1
(2,1013)	1:79:A:ILE:HG12	1:79:A:ILE:HG22	8	0.1
(2,901)	1:79:A:ILE:HD13	1:79:A:ILE:HB	7	0.1
(2,830)	1:20:A:ALA:H	1:20:A:ALA:HB3	8	0.1
(2,826)	1:91:A:LEU:H	1:90:A:ALA:HB1	3	0.1
(2,791)	1:95:A:VAL:HG23	1:95:A:VAL:HB	6	0.1
(2,687)	1:16:A:ARG:HG2	1:16:A:ARG:HB2	9	0.1
(2,674)	1:66:A:ARG:HB2	1:68:A:ARG:HG2	5	0.1
(2,669)	1:70:A:LYS:HD3	1:70:A:LYS:HB2	10	0.1
(2,663)	1:21:A:ARG:HB3	1:22:A:ILE:H	8	0.1
(2,547)	1:70:A:LYS:HE3	1:43:A:PRO:HG2	10	0.1
(2,484)	1:3:A:LYS:HA	1:109:A:THR:HB	6	0.1
(2,475)	1:18:A:GLU:HA	1:22:A:ILE:HG23	1	0.1
(2,473)	1:12:A:LEU:HA	1:12:A:LEU:HG	6	0.1
(2,443)	1:87:A:PRO:HA	1:87:A:PRO:HB2	3	0.1
(2,443)	1:87:A:PRO:HA	1:87:A:PRO:HB2	6	0.1
(2,443)	1:87:A:PRO:HA	1:87:A:PRO:HB2	10	0.1
(2,412)	1:64:A:VAL:HA	1:66:A:ARG:HB3	4	0.1
(2,391)	1:104:A:GLY:H	1:101:A:ASP:HB2	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,346)	1:99:A:LYS:H	1:98:A:GLU:HB2	2	0.1
(2,327)	1:97:A:GLU:H	1:97:A:GLU:HB3	3	0.1
(2,313)	1:79:A:ILE:H	1:79:A:ILE:HG12	3	0.1
(2,268)	1:84:A:VAL:H	1:84:A:VAL:HB	9	0.1
(2,253)	1:113:A:GLU:H	1:115:A:THR:HB	1	0.1
(2,251)	1:80:A:PHE:H	1:111:A:SER:HB2	7	0.1
(2,221)	1:49:A:LYS:H	1:49:A:LYS:HD2	8	0.1
(2,219)	1:49:A:LYS:H	1:48:A:LYS:HB3	6	0.1
(2,219)	1:49:A:LYS:H	1:48:A:LYS:HB3	8	0.1
(2,207)	1:21:A:ARG:H	1:19:A:ALA:HA	4	0.1
(2,205)	1:62:A:VAL:H	1:59:A:GLY:HA3	3	0.1
(2,205)	1:62:A:VAL:H	1:59:A:GLY:HA3	9	0.1
(2,181)	1:100:A:LYS:H	1:100:A:LYS:HG2	3	0.1
(2,121)	1:14:A:LYS:H	1:13:A:GLU:H	10	0.1
(2,119)	1:109:A:THR:H	1:110:A:TYR:H	6	0.1
(2,115)	1:90:A:ALA:H	1:90:A:ALA:HB2	1	0.1
(2,100)	1:95:A:VAL:H	1:94:A:SER:HB3	10	0.1
(2,56)	1:78:A:PHE:H	1:78:A:PHE:HD2	6	0.1
(2,50)	1:108:A:VAL:H	1:109:A:THR:H	3	0.1
(2,33)	1:102:A:ASP:H	1:101:A:ASP:H	3	0.1
(2,10)	1:85:A:LEU:H	1:80:A:PHE:HD1	4	0.1
(1,248)	1:50:A:TYR:HE1	1:32:A:VAL:HB	1	0.1
(1,128)	1:3:A:LYS:HB3	1:35:A:GLU:HB2	3	0.1
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	1	0.1
(1,106)	1:83:A:ASN:HA	1:80:A:PHE:HB3	2	0.1
(1,81)	1:67:A:LYS:HA	1:71:A:LEU:HB2	5	0.1
(1,49)	1:67:A:LYS:H	1:65:A:ILE:H	2	0.1
(1,48)	1:79:A:ILE:H	1:80:A:PHE:H	2	0.1
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG21	4	0.1
(1,47)	1:63:A:TYR:H	1:62:A:VAL:HG21	7	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	1	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	3	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	4	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	5	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	6	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	7	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	8	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	9	0.1
(1,46)	1:24:A:GLU:H	1:24:A:GLU:HA	10	0.1
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	2	0.1
(1,39)	1:20:A:ALA:H	1:21:A:ARG:HB3	7	0.1
(1,35)	1:96:A:TYR:H	1:95:A:VAL:HG11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:109:A:THR:H	1:110:A:TYR:H	7	0.1
(1,29)	1:109:A:THR:H	1:110:A:TYR:H	8	0.1
(1,7)	1:45:A:ILE:H	1:44:A:THR:HA	9	0.1

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

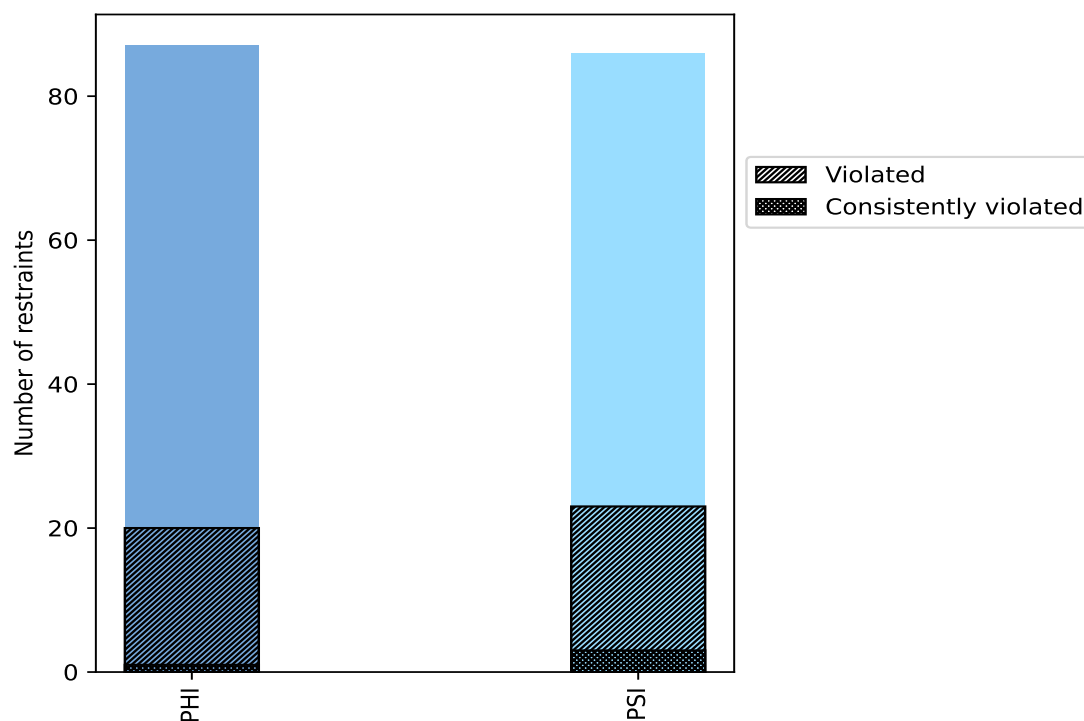
### 10.1 Summary of dihedral-angle violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	87	50.3	20	23.0	11.6	1	1.1	0.6
PSI	86	49.7	23	26.7	13.3	3	3.5	1.7
Total	173	100.0	43	24.9	24.9	4	2.3	2.3

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

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



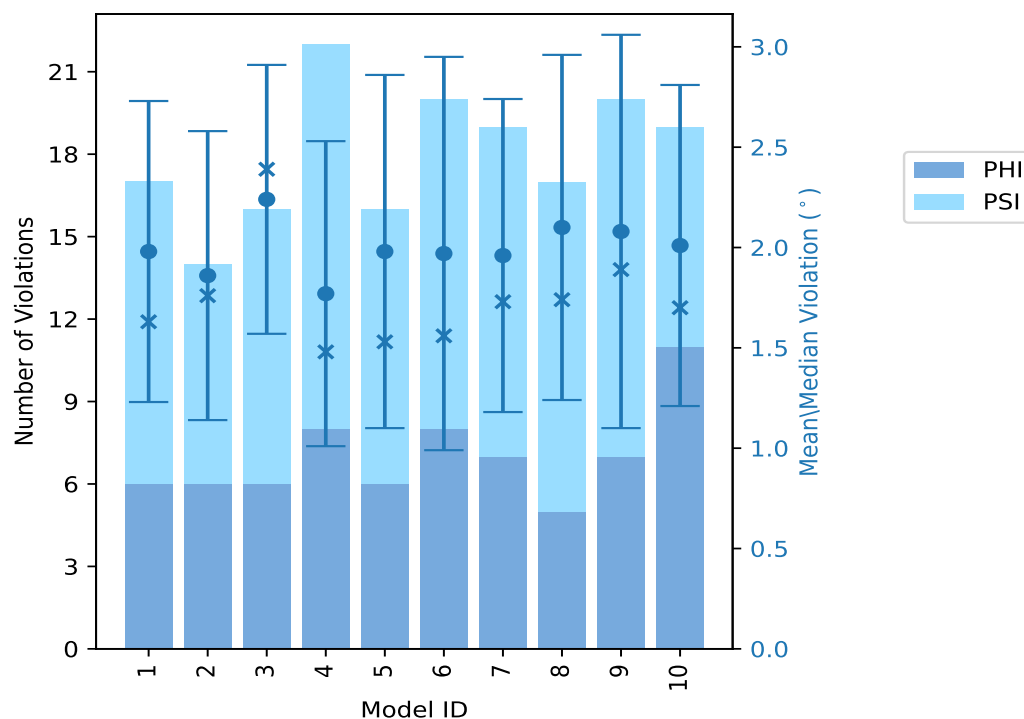
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°)
	PHI	PSI	Total				
1	6	11	17	1.98	3.42	0.75	1.63
2	6	8	14	1.86	3.26	0.72	1.76
3	6	10	16	2.24	3.65	0.67	2.39
4	8	14	22	1.77	3.28	0.76	1.48
5	6	10	16	1.98	3.82	0.88	1.53
6	8	12	20	1.97	4.75	0.98	1.56
7	7	12	19	1.96	3.39	0.78	1.73
8	5	12	17	2.1	3.81	0.86	1.74
9	7	13	20	2.08	4.91	0.98	1.89
10	11	8	19	2.01	3.81	0.8	1.7

### 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

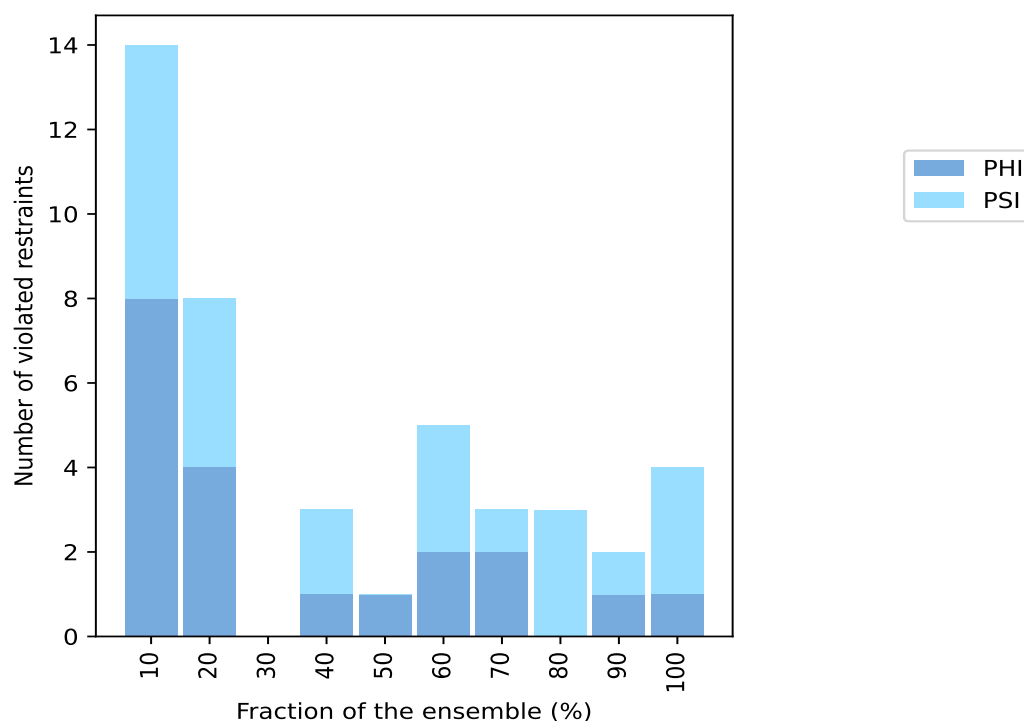
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PHI	PSI	Total	Count <sup>1</sup>	%
8	6	14	1	10.0
4	4	8	2	20.0
0	0	0	3	30.0
1	2	3	4	40.0
1	0	1	5	50.0
2	3	5	6	60.0
2	1	3	7	70.0
0	3	3	8	80.0
1	1	2	9	90.0
1	3	4	10	100.0

<sup>1</sup> Number of models with violations

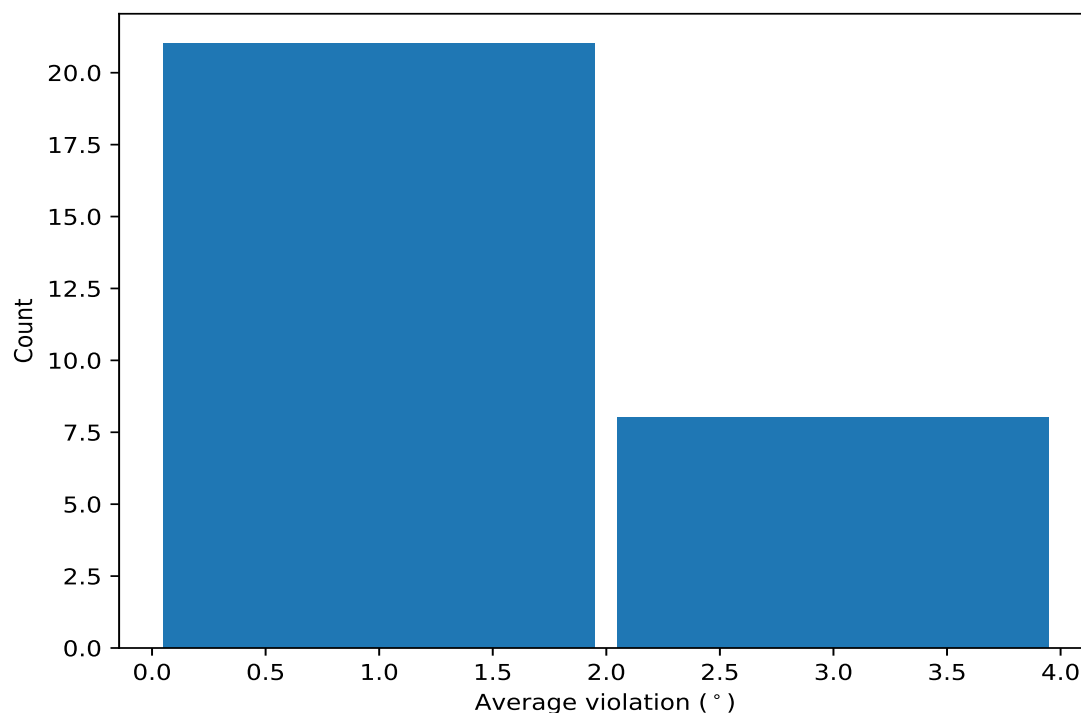
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	10	3.2	0.52	3.34
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	10	2.96	1.15	2.98
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	10	2.88	0.29	2.95
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	10	2.39	0.6	2.3
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	9	1.87	0.43	1.89
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	9	1.86	0.62	1.65
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	8	2.72	0.84	2.66
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	8	1.99	0.57	1.79
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	8	1.71	0.46	1.69
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	7	2.76	0.38	2.69
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	7	1.27	0.13	1.29
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	7	1.24	0.17	1.2
(1,154)	1:100:A:LYS:C	1:101:A:ASP:N	1:101:A:ASP:CA	1:101:A:ASP:C	6	2.48	0.15	2.46

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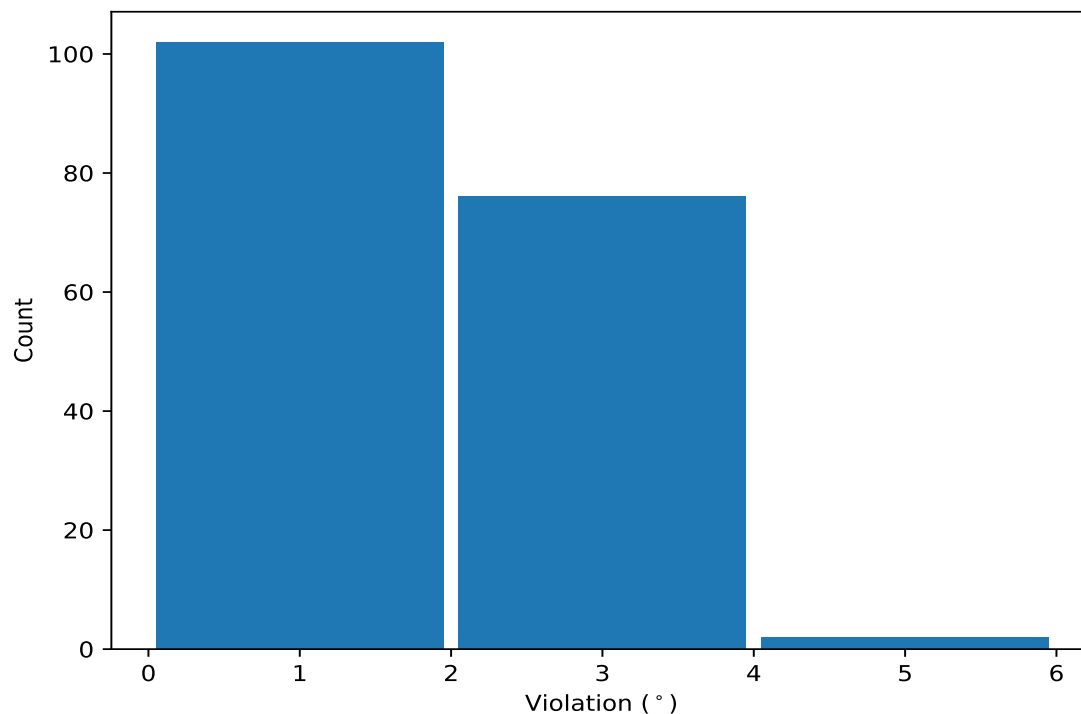
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,45)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	6	2.34	0.83	1.98
(1,40)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:VAL:N	6	1.39	0.32	1.32
(1,92)	1:63:A:TYR:N	1:63:A:TYR:CA	1:63:A:TYR:C	1:64:A:VAL:N	6	1.32	0.12	1.26
(1,139)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:LEU:N	6	1.19	0.1	1.2
(1,146)	1:95:A:VAL:C	1:96:A:TYR:N	1:96:A:TYR:CA	1:96:A:TYR:C	5	1.26	0.16	1.29
(1,63)	1:44:A:THR:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	4	1.71	0.24	1.6
(1,44)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:VAL:N	4	1.38	0.21	1.31
(1,141)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:MET:N	4	1.25	0.2	1.2
(1,165)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:TYR:N	2	1.9	0.01	1.9
(1,162)	1:107:A:TYR:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	2	1.8	0.49	1.8
(1,61)	1:42:A:ILE:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	2	1.75	0.57	1.75
(1,71)	1:49:A:LYS:C	1:50:A:TYR:N	1:50:A:TYR:CA	1:50:A:TYR:C	2	1.46	0.24	1.46
(1,163)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:THR:N	2	1.36	0.27	1.36
(1,2)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:SER:N	2	1.14	0.03	1.14
(1,102)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:ILE:N	2	1.14	0.08	1.14
(1,111)	1:73:A:ALA:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	2	1.06	0.01	1.06

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	9	4.91
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	6	4.75
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	9	3.84
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	5	3.82
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	10	3.81
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	8	3.81
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	6	3.79
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	3	3.65
(1,45)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	10	3.6
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	8	3.54
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	1	3.42
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	5	3.4
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	7	3.39
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	8	3.35
(1,45)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	7	3.35
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	9	3.28
(1,10)	1:10:A:HIS:N	1:10:A:HIS:CA	1:10:A:HIS:C	1:11:A:ASP:N	4	3.28
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	2	3.26
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	6	3.21
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	1	3.19
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	4	3.18
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	5	3.15
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	4	3.07
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	2	3.07
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	10	3.01
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	3	2.96
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	7	2.95
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	4	2.94
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	7	2.89
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	1	2.87
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	6	2.83
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	5	2.8
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	8	2.78
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	10	2.78
(1,154)	1:100:A:LYS:C	1:101:A:ASP:N	1:101:A:ASP:CA	1:101:A:ASP:C	3	2.74
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	7	2.74
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	7	2.69
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	10	2.68
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	3	2.67
(1,19)	1:15:A:ARG:C	1:16:A:ARG:N	1:16:A:ARG:CA	1:16:A:ARG:C	1	2.65
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1	2.62
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	3	2.6
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	4	2.58
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	8	2.58
(1,154)	1:100:A:LYS:C	1:101:A:ASP:N	1:101:A:ASP:CA	1:101:A:ASP:C	2	2.56
(1,154)	1:100:A:LYS:C	1:101:A:ASP:N	1:101:A:ASP:CA	1:101:A:ASP:C	6	2.56
(1,121)	1:78:A:PHE:C	1:79:A:ILE:N	1:79:A:ILE:CA	1:79:A:ILE:C	9	2.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	3	2.53
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	3	2.52
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	9	2.49
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	5	2.49
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	8	2.46
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	1	2.46
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	3	2.44
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	8	2.4
(1,66)	1:46:A:ASP:N	1:46:A:ASP:CA	1:46:A:ASP:C	1:47:A:LYS:N	9	2.39
(1,154)	1:100:A:LYS:C	1:101:A:ASP:N	1:101:A:ASP:CA	1:101:A:ASP:C	1	2.37
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	2	2.36
(1,154)	1:100:A:LYS:C	1:101:A:ASP:N	1:101:A:ASP:CA	1:101:A:ASP:C	9	2.35
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	3	2.34
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	4	2.32
(1,61)	1:42:A:ILE:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	6	2.32
(1,154)	1:100:A:LYS:C	1:101:A:ASP:N	1:101:A:ASP:CA	1:101:A:ASP:C	10	2.31
(1,162)	1:107:A:TYR:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	8	2.3
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	5	2.29
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	2	2.27
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	7	2.26
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	9	2.22
(1,60)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	9	2.2
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	3	2.19
(1,45)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	3	2.16
(1,63)	1:44:A:THR:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	10	2.12
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	4	2.06
(1,172)	1:112:A:GLY:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	6	2.04
(1,99)	1:66:A:ARG:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	5	2.02
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	10	2.01
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	7	2.0
(1,105)	1:70:A:LYS:C	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	9	2.0
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	6	1.97
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	1	1.96
(1,165)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:TYR:N	4	1.9
(1,165)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:TYR:N	2	1.89
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	10	1.89
(1,40)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:VAL:N	3	1.88
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	7	1.85
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	2	1.83
(1,45)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	6	1.8
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	9	1.78
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	9	1.75
(1,40)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:VAL:N	8	1.74
(1,44)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:VAL:N	7	1.73
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	10	1.7
(1,71)	1:49:A:LYS:C	1:50:A:TYR:N	1:50:A:TYR:CA	1:50:A:TYR:C	2	1.7
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	4	1.69
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	10	1.65
(1,45)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	8	1.65
(1,163)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:THR:N	1	1.63
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	1	1.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	6	1.61
(1,63)	1:44:A:THR:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	7	1.61
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	8	1.6
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	5	1.58
(1,63)	1:44:A:THR:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	9	1.58
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	3	1.58
(1,141)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:MET:N	4	1.55
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	10	1.55
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	10	1.55
(1,63)	1:44:A:THR:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	8	1.53
(1,68)	1:47:A:LYS:N	1:47:A:LYS:CA	1:47:A:LYS:C	1:48:A:LYS:N	10	1.51
(1,92)	1:63:A:TYR:N	1:63:A:TYR:CA	1:63:A:TYR:C	1:64:A:VAL:N	6	1.5
(1,146)	1:95:A:VAL:C	1:96:A:TYR:N	1:96:A:TYR:CA	1:96:A:TYR:C	4	1.49
(1,92)	1:63:A:TYR:N	1:63:A:TYR:CA	1:63:A:TYR:C	1:64:A:VAL:N	5	1.48
(1,45)	1:33:A:ILE:C	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	4	1.48
(1,166)	1:109:A:THR:C	1:110:A:TYR:N	1:110:A:TYR:CA	1:110:A:TYR:C	2	1.47
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	6	1.46
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	6	1.46
(1,173)	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1:114:A:ASN:N	1	1.45
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	5	1.36
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	7	1.36
(1,62)	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	1:44:A:THR:N	4	1.35
(1,40)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:VAL:N	9	1.35
(1,146)	1:95:A:VAL:C	1:96:A:TYR:N	1:96:A:TYR:CA	1:96:A:TYR:C	7	1.34
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	6	1.34
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	6	1.32
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	10	1.32
(1,162)	1:107:A:TYR:C	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	10	1.31
(1,141)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:MET:N	7	1.31
(1,139)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:LEU:N	4	1.31
(1,44)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:VAL:N	1	1.31
(1,169)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:GLY:N	8	1.3
(1,139)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:LEU:N	5	1.3
(1,44)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:VAL:N	9	1.3
(1,146)	1:95:A:VAL:C	1:96:A:TYR:N	1:96:A:TYR:CA	1:96:A:TYR:C	5	1.29
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	8	1.29
(1,92)	1:63:A:TYR:N	1:63:A:TYR:CA	1:63:A:TYR:C	1:64:A:VAL:N	7	1.29
(1,40)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:VAL:N	1	1.29
(1,1)	1:3:A:LYS:C	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	2	1.29
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	1	1.26
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1	1.24
(1,139)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:LEU:N	6	1.23
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	5	1.23
(1,132)	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	1:85:A:LEU:N	9	1.23
(1,92)	1:63:A:TYR:N	1:63:A:TYR:CA	1:63:A:TYR:C	1:64:A:VAL:N	3	1.23
(1,102)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:ILE:N	9	1.22
(1,92)	1:63:A:TYR:N	1:63:A:TYR:CA	1:63:A:TYR:C	1:64:A:VAL:N	4	1.22
(1,92)	1:63:A:TYR:N	1:63:A:TYR:CA	1:63:A:TYR:C	1:64:A:VAL:N	1	1.21
(1,71)	1:49:A:LYS:C	1:50:A:TYR:N	1:50:A:TYR:CA	1:50:A:TYR:C	4	1.21
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	5	1.2
(1,61)	1:42:A:ILE:C	1:43:A:PRO:N	1:43:A:PRO:CA	1:43:A:PRO:C	10	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:SER:N	3	1.18
(1,139)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:LEU:N	8	1.17
(1,106)	1:71:A:LEU:N	1:71:A:LEU:CA	1:71:A:LEU:C	1:72:A:SER:N	5	1.17
(1,44)	1:33:A:ILE:N	1:33:A:ILE:CA	1:33:A:ILE:C	1:34:A:VAL:N	6	1.17
(1,18)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	7	1.17
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	3	1.15
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	7	1.14
(1,158)	1:105:A:PHE:C	1:106:A:LEU:N	1:106:A:LEU:CA	1:106:A:LEU:C	1	1.11
(1,146)	1:95:A:VAL:C	1:96:A:TYR:N	1:96:A:TYR:CA	1:96:A:TYR:C	8	1.11
(1,2)	1:4:A:SER:N	1:4:A:SER:CA	1:4:A:SER:C	1:5:A:SER:N	9	1.11
(1,40)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:VAL:N	2	1.1
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	4	1.1
(1,163)	1:108:A:VAL:N	1:108:A:VAL:CA	1:108:A:VAL:C	1:109:A:THR:N	4	1.09
(1,22)	1:17:A:ALA:N	1:17:A:ALA:CA	1:17:A:ALA:C	1:18:A:GLU:N	7	1.09
(1,141)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:MET:N	8	1.08
(1,141)	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	1:92:A:MET:N	2	1.07
(1,139)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:LEU:N	7	1.07
(1,111)	1:73:A:ALA:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	4	1.07
(1,108)	1:72:A:SER:N	1:72:A:SER:CA	1:72:A:SER:C	1:73:A:ALA:N	9	1.07
(1,146)	1:95:A:VAL:C	1:96:A:TYR:N	1:96:A:TYR:CA	1:96:A:TYR:C	10	1.06
(1,111)	1:73:A:ALA:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	10	1.06
(1,102)	1:68:A:ARG:N	1:68:A:ARG:CA	1:68:A:ARG:C	1:69:A:ILE:N	6	1.06
(1,50)	1:36:A:LYS:N	1:36:A:LYS:CA	1:36:A:LYS:C	1:37:A:ALA:N	9	1.06
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	2	1.06
(1,139)	1:90:A:ALA:N	1:90:A:ALA:CA	1:90:A:ALA:C	1:91:A:LEU:N	2	1.05
(1,128)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:ASN:N	4	1.04
(1,117)	1:76:A:ALA:C	1:77:A:ILE:N	1:77:A:ILE:CA	1:77:A:ILE:C	5	1.03
(1,47)	1:34:A:VAL:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	6	1.03
(1,31)	1:21:A:ARG:C	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	4	1.02
(1,135)	1:85:A:LEU:C	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	4	1.01
(1,40)	1:31:A:PRO:N	1:31:A:PRO:CA	1:31:A:PRO:C	1:32:A:VAL:N	6	1.0