



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 12:08 PM UTC

PDB ID : 2LBF / pdb\_00002lbf  
Title : Solution structure of the dimerization domain of human ribosomal protein P1/P2 heterodimer  
Authors : Lee, K.-M.; Yu, C.W.-H.; Chiu, T.Y.-H.; Sze, K.-H.; Shaw, P.-C.; Wong, K.-B.  
Deposited on : 2011-03-30

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 : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

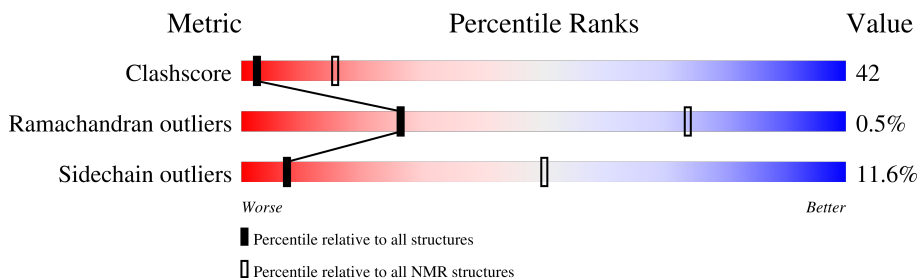
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 69%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	69	
2	B	70	

## 2 Ensemble composition and analysis i

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:3-A:60, B:103-B:160 (116)	0.33	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 5 single-model clusters were found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 2031 atoms, of which 1029 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 60S acidic ribosomal protein P1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	69	1002	318	505	80	96	3	0

- Molecule 2 is a protein called 60S acidic ribosomal protein P2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	70	1029	314	524	87	103	1	0

There is a discrepancy between the modelled and reference sequences:

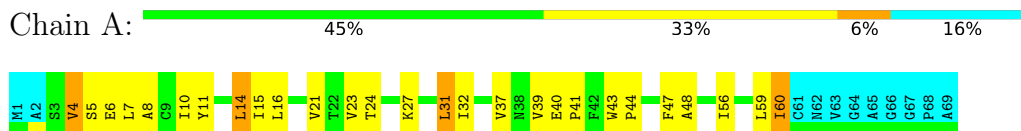
Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ALA	-	expression tag	UNP P05387

## 4 Residue-property plots [i](#)

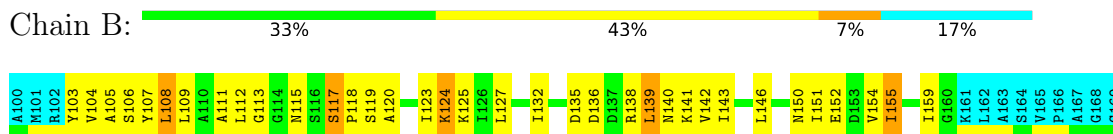
### 4.1 Average score per residue in the NMR ensemble

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: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2

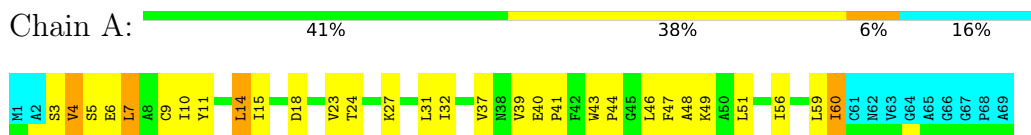


### 4.2 Scores per residue for each member of the ensemble

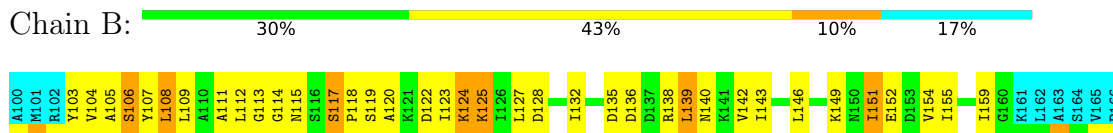
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2



A167  
G168  
G169

#### 4.2.2 Score per residue for model 2

- Molecule 1: 60S acidic ribosomal protein P1

Chain A: 43% 32% 9% 16%



- Molecule 2: 60S acidic ribosomal protein P2

Chain B: 33% 41% 9% 17%



#### 4.2.3 Score per residue for model 3

- Molecule 1: 60S acidic ribosomal protein P1

Chain A: 43% 36% 16%



- Molecule 2: 60S acidic ribosomal protein P2

Chain B: 33% 40% 10% 17%



#### 4.2.4 Score per residue for model 4

- Molecule 1: 60S acidic ribosomal protein P1

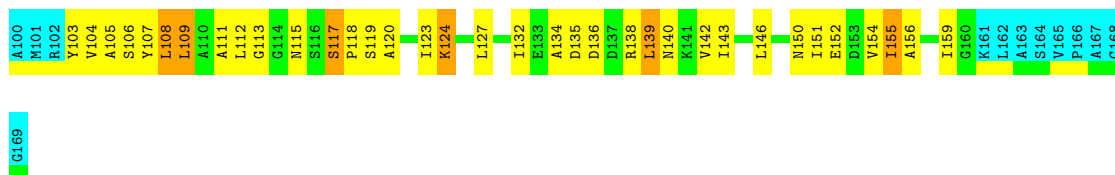
Chain A: 42% 38% 16%



- Molecule 2: 60S acidic ribosomal protein P2

Chain B: 33% 41% 9% 17%





#### 4.2.5 Score per residue for model 5

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2

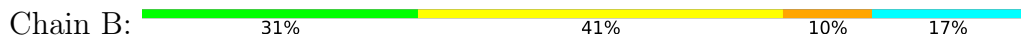


#### 4.2.6 Score per residue for model 6

- Molecule 1: 60S acidic ribosomal protein P1

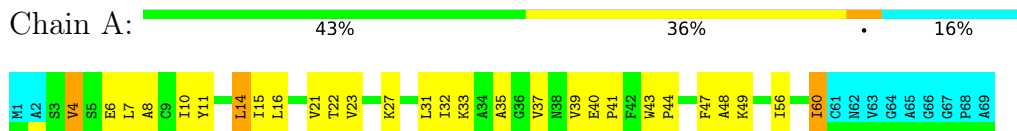


- Molecule 2: 60S acidic ribosomal protein P2

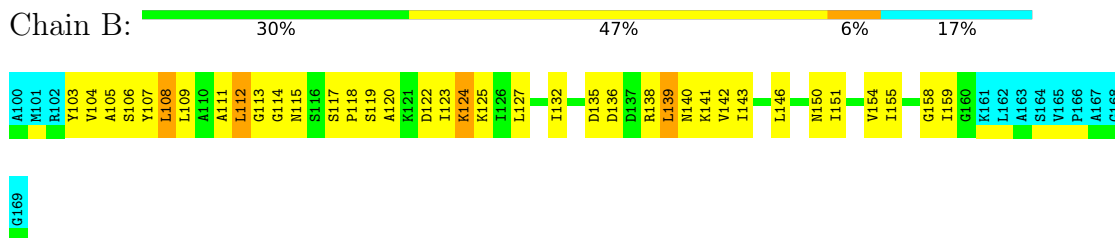


#### 4.2.7 Score per residue for model 7

- Molecule 1: 60S acidic ribosomal protein P1

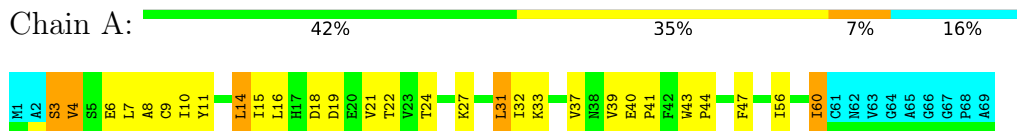


- Molecule 2: 60S acidic ribosomal protein P2

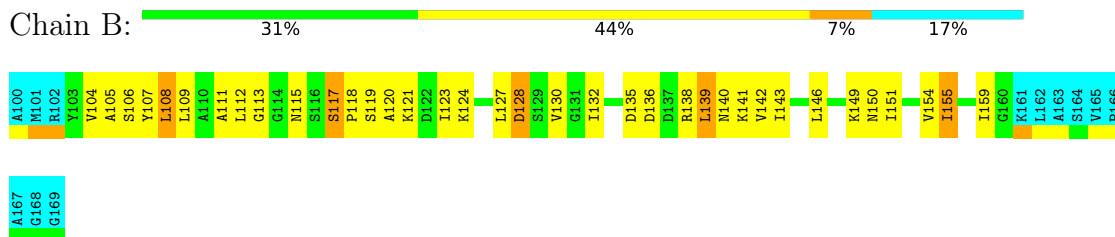


#### 4.2.8 Score per residue for model 8

- Molecule 1: 60S acidic ribosomal protein P1

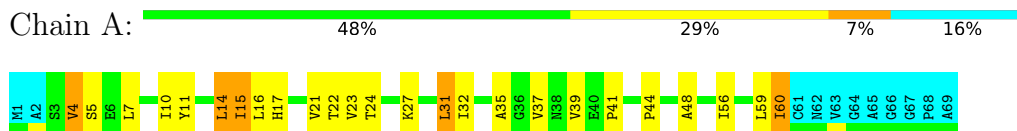


- Molecule 2: 60S acidic ribosomal protein P2



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

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2



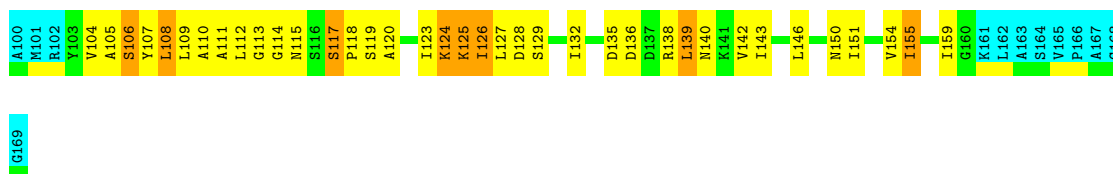


#### 4.2.10 Score per residue for model 10

- Molecule 1: 60S acidic ribosomal protein P1



- Molecule 2: 60S acidic ribosomal protein P2



## 5 Refinement protocol and experimental data overview

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

Of the 100 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	

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	1202
Number of shifts mapped to atoms	1202
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	69%

## 6 Model quality i

### 6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.58±0.02	0±0/441 ( 0.0± 0.0%)	0.90±0.01	0±0/604 ( 0.0± 0.0%)
2	B	0.61±0.02	0±0/428 ( 0.0± 0.0%)	0.94±0.03	2±1/578 ( 0.3± 0.1%)
All	All	0.60	0/8690 ( 0.0%)	0.92	18/11820 ( 0.2%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	117	SER	CA-C-N	5.45	125.44	120.21	9	9
2	B	117	SER	C-N-CA	5.45	125.44	120.21	9	9

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	433	443	442	32±2
2	B	425	434	434	56±4
All	All	8580	8770	8760	737

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 43.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:136:ASP:HA	2:B:139:LEU:HD11	0.90	1.36	6	10
1:A:37:VAL:HB	2:B:113:GLY:HA3	0.88	1.43	1	2
2:B:103:TYR:HB2	2:B:142:VAL:HG11	0.81	1.51	1	7
1:A:4:VAL:HG13	2:B:112:LEU:HG	0.80	1.53	2	10
2:B:124:LYS:HD2	2:B:127:LEU:HD11	0.80	1.53	6	2
1:A:37:VAL:HB	2:B:113:GLY:HA2	0.80	1.52	7	8
2:B:139:LEU:O	2:B:143:ILE:HG12	0.79	1.76	6	6
1:A:7:LEU:HD12	1:A:10:ILE:HD12	0.75	1.57	9	10
2:B:127:LEU:HB2	2:B:132:ILE:HB	0.73	1.60	5	2
1:A:60:ILE:HG13	2:B:159:ILE:HB	0.73	1.60	10	9
2:B:120:ALA:HB1	2:B:139:LEU:HD13	0.72	1.59	2	10
2:B:154:VAL:HB	2:B:155:ILE:HD12	0.72	1.62	8	10
1:A:11:TYR:HB2	2:B:109:LEU:HD13	0.71	1.62	1	9
2:B:108:LEU:HD12	2:B:151:ILE:HG13	0.71	1.62	6	10
2:B:111:ALA:HA	2:B:115:ASN:O	0.71	1.85	10	10
1:A:5:SER:HB3	1:A:39:VAL:HA	0.71	1.62	9	6
1:A:14:LEU:HD22	1:A:56:ILE:HD11	0.71	1.61	2	10
1:A:7:LEU:HA	1:A:10:ILE:HD12	0.69	1.64	3	10
2:B:106:SER:HB2	2:B:123:ILE:HG23	0.69	1.64	6	10
2:B:135:ASP:HB2	2:B:138:ARG:HG3	0.68	1.66	10	8
2:B:124:LYS:HD3	2:B:139:LEU:HD21	0.67	1.65	3	8
2:B:107:TYR:O	2:B:118:PRO:HG2	0.66	1.90	3	10
1:A:59:LEU:HB2	2:B:159:ILE:HG21	0.66	1.66	1	8
2:B:123:ILE:CG1	2:B:143:ILE:HD11	0.66	2.21	1	7
2:B:135:ASP:HB2	2:B:138:ARG:CG	0.65	2.21	9	9
1:A:19:ASP:HB2	2:B:132:ILE:HG23	0.65	1.69	8	4
2:B:123:ILE:O	2:B:127:LEU:HG	0.65	1.92	1	9
1:A:24:THR:OG1	1:A:27:LYS:HG2	0.64	1.92	2	1
2:B:108:LEU:HG	2:B:155:ILE:CD1	0.62	2.24	7	10
1:A:15:ILE:HD11	2:B:109:LEU:HD12	0.62	1.71	4	1
1:A:7:LEU:O	1:A:10:ILE:HB	0.61	1.95	7	10
2:B:155:ILE:O	2:B:159:ILE:HD12	0.61	1.96	1	1
2:B:107:TYR:HD2	2:B:143:ILE:HG12	0.61	1.56	4	3
2:B:122:ASP:HA	2:B:125:LYS:HE3	0.61	1.73	5	1
2:B:142:VAL:O	2:B:146:LEU:HG	0.61	1.95	2	5
2:B:140:ASN:O	2:B:143:ILE:HB	0.60	1.95	7	6
2:B:123:ILE:HG13	2:B:143:ILE:HD11	0.60	1.73	4	4
1:A:16:LEU:HD12	1:A:21:VAL:HG13	0.60	1.74	5	4
2:B:107:TYR:CG	2:B:146:LEU:HD12	0.60	2.30	8	5
2:B:108:LEU:HG	2:B:155:ILE:HD13	0.60	1.73	9	9
1:A:21:VAL:HG22	1:A:22:THR:H	0.60	1.57	9	3
1:A:5:SER:HB2	1:A:39:VAL:HA	0.59	1.74	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:107:TYR:CD2	2:B:143:ILE:HG12	0.59	2.32	4	4
2:B:155:ILE:HD12	2:B:155:ILE:N	0.59	2.13	5	10
2:B:130:VAL:HG23	2:B:132:ILE:HG13	0.59	1.72	8	1
2:B:111:ALA:HB3	2:B:151:ILE:HG12	0.58	1.75	1	5
1:A:11:TYR:OH	2:B:155:ILE:HB	0.58	1.99	5	9
2:B:139:LEU:O	2:B:142:VAL:HG12	0.58	1.99	2	10
1:A:11:TYR:CE2	2:B:112:LEU:HD22	0.57	2.34	1	3
1:A:60:ILE:CD1	2:B:159:ILE:HB	0.57	2.29	3	9
1:A:60:ILE:CG1	2:B:159:ILE:HB	0.57	2.28	10	6
2:B:146:LEU:O	2:B:149:LYS:HB2	0.57	2.00	8	2
1:A:14:LEU:HB3	2:B:105:ALA:CB	0.57	2.30	7	10
2:B:108:LEU:HG	2:B:155:ILE:HD11	0.57	1.77	1	1
2:B:125:LYS:HD2	2:B:126:ILE:HD12	0.57	1.76	10	2
1:A:3:SER:HB2	1:A:6:GLU:HG3	0.56	1.78	3	2
2:B:112:LEU:HD11	2:B:152:GLU:HG3	0.56	1.77	5	4
1:A:37:VAL:HB	2:B:113:GLY:CA	0.56	2.25	1	9
2:B:115:ASN:C	2:B:117:SER:H	0.56	2.08	10	10
1:A:31:LEU:HB3	2:B:109:LEU:HD21	0.56	1.76	9	6
2:B:107:TYR:CZ	2:B:118:PRO:HD2	0.56	2.36	1	10
2:B:138:ARG:O	2:B:141:LYS:HG3	0.56	2.01	3	1
1:A:32:ILE:HG23	1:A:37:VAL:O	0.55	2.01	4	10
1:A:37:VAL:HG21	2:B:112:LEU:HB3	0.55	1.76	10	2
2:B:119:SER:O	2:B:123:ILE:HG12	0.55	2.01	7	9
2:B:135:ASP:HB3	2:B:138:ARG:HG3	0.54	1.79	6	1
1:A:7:LEU:HD11	2:B:155:ILE:O	0.54	2.02	4	3
2:B:106:SER:CB	2:B:123:ILE:HG23	0.54	2.32	9	9
2:B:138:ARG:HA	2:B:141:LYS:HE2	0.53	1.80	6	1
2:B:139:LEU:O	2:B:143:ILE:HD12	0.53	2.03	3	4
2:B:135:ASP:HB3	2:B:138:ARG:CG	0.53	2.33	6	1
2:B:104:VAL:HA	2:B:146:LEU:HD11	0.53	1.81	9	2
2:B:138:ARG:O	2:B:141:LYS:HG2	0.53	2.03	6	3
2:B:139:LEU:HA	2:B:142:VAL:HG12	0.53	1.81	4	7
2:B:105:ALA:HA	2:B:108:LEU:HD22	0.52	1.80	9	5
1:A:47:PHE:HD2	1:A:51:LEU:HD11	0.52	1.65	4	2
2:B:141:LYS:O	2:B:145:GLU:HG2	0.52	2.05	2	1
2:B:121:LYS:HD2	2:B:121:LYS:N	0.51	2.20	6	3
1:A:23:VAL:HG12	1:A:48:ALA:HA	0.51	1.81	10	6
2:B:122:ASP:O	2:B:125:LYS:HB2	0.51	2.04	7	1
2:B:115:ASN:ND2	2:B:118:PRO:HA	0.51	2.19	3	5
2:B:124:LYS:CD	2:B:139:LEU:HD21	0.51	2.35	2	3
2:B:123:ILE:HG22	2:B:127:LEU:HD23	0.51	1.82	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:GLU:HG2	1:A:43:TRP:NE1	0.50	2.22	10	3
2:B:139:LEU:HD12	2:B:140:ASN:H	0.50	1.65	10	5
2:B:136:ASP:CA	2:B:139:LEU:HD11	0.50	2.24	6	3
2:B:135:ASP:O	2:B:139:LEU:HG	0.50	2.07	6	6
2:B:119:SER:C	2:B:143:ILE:HD13	0.50	2.31	1	4
2:B:150:ASN:O	2:B:154:VAL:HG23	0.50	2.06	6	8
2:B:104:VAL:O	2:B:108:LEU:HD22	0.49	2.07	6	7
1:A:8:ALA:HB2	2:B:112:LEU:HD23	0.49	1.82	7	6
1:A:50:ALA:O	1:A:54:VAL:HG22	0.49	2.07	2	1
1:A:43:TRP:CE3	1:A:47:PHE:HE1	0.49	2.25	1	5
2:B:120:ALA:HB1	2:B:139:LEU:CD1	0.49	2.36	6	4
1:A:24:THR:OG1	1:A:27:LYS:HB2	0.49	2.07	4	4
2:B:107:TYR:CZ	2:B:146:LEU:HB3	0.48	2.42	6	4
2:B:107:TYR:CE1	2:B:118:PRO:HD2	0.48	2.43	8	1
1:A:10:ILE:HD13	2:B:159:ILE:CG1	0.48	2.38	5	3
1:A:47:PHE:CD2	1:A:51:LEU:HD11	0.48	2.43	1	1
1:A:7:LEU:HB3	2:B:112:LEU:HD21	0.48	1.84	1	3
1:A:16:LEU:HD21	1:A:23:VAL:HA	0.48	1.85	6	2
1:A:29:ASN:HA	1:A:32:ILE:HD12	0.48	1.84	5	1
1:A:40:GLU:HB2	1:A:43:TRP:CD1	0.48	2.44	6	2
1:A:34:ALA:HB1	2:B:126:ILE:HA	0.48	1.85	10	2
2:B:135:ASP:OD1	2:B:138:ARG:HG2	0.48	2.08	6	1
2:B:139:LEU:HD12	2:B:140:ASN:N	0.48	2.24	8	4
2:B:155:ILE:HG22	2:B:155:ILE:O	0.48	2.08	10	5
1:A:10:ILE:HD13	2:B:159:ILE:HG13	0.47	1.85	2	3
2:B:117:SER:N	2:B:118:PRO:HD3	0.47	2.24	4	10
1:A:21:VAL:HG22	1:A:22:THR:N	0.47	2.24	9	4
1:A:37:VAL:CG1	2:B:109:LEU:HD23	0.47	2.40	4	1
1:A:11:TYR:HA	1:A:14:LEU:HB2	0.47	1.86	3	8
1:A:24:THR:OG1	1:A:27:LYS:HE2	0.47	2.10	8	3
2:B:124:LYS:O	2:B:128:ASP:HB2	0.47	2.10	10	4
2:B:155:ILE:O	2:B:155:ILE:HG22	0.47	2.09	7	4
1:A:7:LEU:HD12	1:A:10:ILE:CD1	0.47	2.34	9	2
1:A:11:TYR:CE1	2:B:155:ILE:HG12	0.47	2.45	1	1
1:A:7:LEU:HD22	2:B:152:GLU:OE1	0.47	2.09	6	1
1:A:11:TYR:HE2	2:B:112:LEU:HD22	0.47	1.70	1	1
2:B:123:ILE:HG12	2:B:143:ILE:HD11	0.47	1.87	1	1
1:A:10:ILE:HG22	1:A:14:LEU:HD23	0.47	1.87	7	5
2:B:103:TYR:HB3	2:B:123:ILE:HG21	0.46	1.85	6	3
1:A:43:TRP:CE3	1:A:47:PHE:CE1	0.46	3.03	1	3
1:A:46:LEU:O	1:A:49:LYS:HB2	0.46	2.11	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:125:LYS:CD	2:B:126:ILE:HD12	0.46	2.40	10	2
1:A:41:PRO:C	1:A:44:PRO:HD2	0.46	2.35	7	7
2:B:146:LEU:O	2:B:149:LYS:HE2	0.46	2.11	1	1
1:A:14:LEU:CD1	1:A:56:ILE:HG12	0.46	2.41	6	7
2:B:142:VAL:O	2:B:146:LEU:HD23	0.46	2.11	1	2
1:A:11:TYR:O	1:A:15:ILE:HG12	0.46	2.11	9	4
2:B:104:VAL:O	2:B:107:TYR:HB3	0.45	2.11	4	5
2:B:104:VAL:HG12	2:B:146:LEU:HD21	0.45	1.88	5	1
1:A:9:CYS:HB2	1:A:39:VAL:HG11	0.45	1.88	8	3
1:A:39:VAL:HG12	1:A:40:GLU:N	0.45	2.26	7	6
1:A:12:SER:HB2	1:A:28:ILE:HG23	0.45	1.89	4	1
2:B:104:VAL:HG12	2:B:108:LEU:HD21	0.45	1.89	9	2
1:A:10:ILE:HG22	1:A:14:LEU:CD2	0.45	2.42	9	1
2:B:140:ASN:HA	2:B:143:ILE:CG1	0.45	2.42	5	2
2:B:107:TYR:CD1	2:B:146:LEU:HD12	0.44	2.47	2	2
1:A:35:ALA:CB	2:B:109:LEU:HG	0.44	2.42	7	2
2:B:124:LYS:HA	2:B:127:LEU:HD11	0.44	1.89	7	2
2:B:127:LEU:HD13	2:B:132:ILE:O	0.44	2.12	7	4
2:B:124:LYS:CD	2:B:127:LEU:HD11	0.44	2.35	6	1
2:B:111:ALA:HA	2:B:115:ASN:C	0.44	2.38	9	3
1:A:6:GLU:O	1:A:10:ILE:HG13	0.44	2.13	3	6
1:A:16:LEU:CD1	1:A:21:VAL:HG13	0.44	2.41	5	1
2:B:104:VAL:HG12	2:B:108:LEU:CD2	0.44	2.43	10	5
1:A:49:LYS:HD2	1:A:49:LYS:O	0.43	2.13	6	1
1:A:3:SER:HB2	1:A:6:GLU:OE1	0.43	2.14	8	1
2:B:110:ALA:HB3	2:B:118:PRO:HB3	0.43	1.90	10	1
2:B:140:ASN:HA	2:B:143:ILE:HG12	0.43	1.91	7	3
1:A:40:GLU:HB3	1:A:43:TRP:HD1	0.43	1.74	7	1
1:A:5:SER:O	1:A:39:VAL:HG22	0.43	2.14	4	2
1:A:27:LYS:O	1:A:31:LEU:HD22	0.43	2.13	6	1
1:A:4:VAL:HG13	2:B:112:LEU:CG	0.43	2.37	2	1
1:A:11:TYR:CD2	2:B:112:LEU:HD22	0.43	2.49	3	1
1:A:31:LEU:HD12	2:B:126:ILE:HG23	0.43	1.91	6	2
2:B:108:LEU:HD12	2:B:151:ILE:CG1	0.43	2.41	8	2
1:A:49:LYS:HD2	1:A:49:LYS:C	0.42	2.38	7	2
2:B:123:ILE:HB	2:B:139:LEU:HD22	0.42	1.91	9	1
1:A:11:TYR:CE2	2:B:108:LEU:HB3	0.42	2.49	4	3
1:A:37:VAL:CB	2:B:113:GLY:HA2	0.42	2.39	9	1
1:A:16:LEU:HD12	1:A:21:VAL:CG1	0.42	2.43	5	1
1:A:24:THR:OG1	1:A:27:LYS:HD2	0.42	2.14	6	1
1:A:32:ILE:HG23	1:A:38:ASN:HA	0.42	1.92	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ILE:HG22	1:A:33:LYS:HD2	0.42	1.90	8	1
2:B:138:ARG:O	2:B:141:LYS:HB3	0.41	2.14	9	1
2:B:115:ASN:C	2:B:117:SER:N	0.41	2.77	10	1
1:A:11:TYR:CB	2:B:109:LEU:HD13	0.41	2.40	9	1
1:A:6:GLU:HG2	1:A:43:TRP:HE1	0.41	1.74	10	2
1:A:40:GLU:O	1:A:43:TRP:HB2	0.41	2.14	6	2
1:A:5:SER:CB	1:A:39:VAL:HA	0.41	2.44	1	1
2:B:111:ALA:CB	2:B:151:ILE:HG12	0.41	2.45	1	2
2:B:155:ILE:HG23	2:B:159:ILE:HA	0.41	1.92	4	1
1:A:17:HIS:CD2	1:A:56:ILE:HB	0.41	2.50	9	1
1:A:16:LEU:HD11	1:A:27:LYS:HG2	0.41	1.93	7	2
2:B:151:ILE:HG22	2:B:152:GLU:N	0.41	2.29	1	1
1:A:22:THR:O	1:A:27:LYS:HG3	0.41	2.16	2	1
2:B:120:ALA:O	2:B:124:LYS:HG2	0.41	2.15	4	1
2:B:127:LEU:HD12	2:B:128:ASP:N	0.41	2.31	8	1
2:B:159:ILE:N	2:B:159:ILE:HD12	0.41	2.31	10	1
2:B:108:LEU:CG	2:B:155:ILE:HD11	0.41	2.43	1	1
2:B:122:ASP:O	2:B:125:LYS:HB3	0.41	2.15	1	1
2:B:106:SER:HB2	2:B:123:ILE:HD12	0.40	1.91	1	1
2:B:103:TYR:OH	2:B:134:ALA:HA	0.40	2.16	4	1
1:A:16:LEU:HD12	1:A:16:LEU:HA	0.40	1.72	9	1
1:A:7:LEU:HD22	2:B:152:GLU:CD	0.40	2.41	1	1
1:A:34:ALA:HB2	2:B:129:SER:CB	0.40	2.46	10	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	58/69 (84%)	54±1 (93±3%)	4±1 (7±3%)	0±0 (0±0%)	100	100
2	B	58/70 (83%)	49±2 (84±3%)	9±2 (15±4%)	1±1 (1±1%)	15	65
All	All	1160/1390 (83%)	1026 (88%)	128 (11%)	6 (1%)	26	74

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	114	GLY	5
2	B	151	ILE	1

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	47/52 (90%)	42±1 (88±1%)	6±1 (12±1%)	<b>7</b> 50
2	B	46/53 (87%)	41±1 (88±2%)	5±1 (12±2%)	<b>8</b> 50
All	All	930/1050 (89%)	822 (88%)	108 (12%)	<b>7</b> 50

All 26 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	14	LEU	10
1	A	15	ILE	10
1	A	31	LEU	10
1	A	60	ILE	10
2	B	108	LEU	10
2	B	139	LEU	10
1	A	4	VAL	9
2	B	124	LYS	7
2	B	155	ILE	7
2	B	106	SER	4
2	B	125	LYS	3
2	B	141	LYS	2
2	B	112	LEU	2
2	B	146	LEU	2
1	A	7	LEU	1
1	A	26	ASP	1
1	A	27	LYS	1
2	B	127	LEU	1
1	A	16	LEU	1
2	B	109	LEU	1
2	B	116	SER	1
1	A	33	LYS	1
1	A	3	SER	1

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Mol	Chain	Res	Type	Models (Total)
2	B	128	ASP	1
2	B	132	ILE	1
2	B	126	ILE	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 69% for the well-defined parts and 68% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping 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	1202
Number of shifts mapped to atoms	1202
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	138	$-0.38 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	122	$0.06 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	0	—	None (insufficient data)

#### 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 69%, i.e. 1048 atoms were assigned a chemical shift out of a possible 1510. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	338/583 (58%)	222/238 (93%)	116/232 (50%)	0/113 (0%)
Sidechain	692/860 (80%)	461/567 (81%)	231/273 (85%)	0/20 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	18/67 (27%)	18/32 (56%)	0/32 (0%)	0/3 (0%)
Overall	1048/1510 (69%)	701/837 (84%)	347/537 (65%)	0/136 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 1202 atoms were assigned a chemical shift out of a possible 1765. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	399/699 (57%)	261/287 (91%)	138/278 (50%)	0/134 (0%)
Sidechain	785/999 (79%)	522/661 (79%)	263/313 (84%)	0/25 (0%)
Aromatic	18/67 (27%)	18/32 (56%)	0/32 (0%)	0/3 (0%)
Overall	1202/1765 (68%)	801/980 (82%)	401/623 (64%)	0/162 (0%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

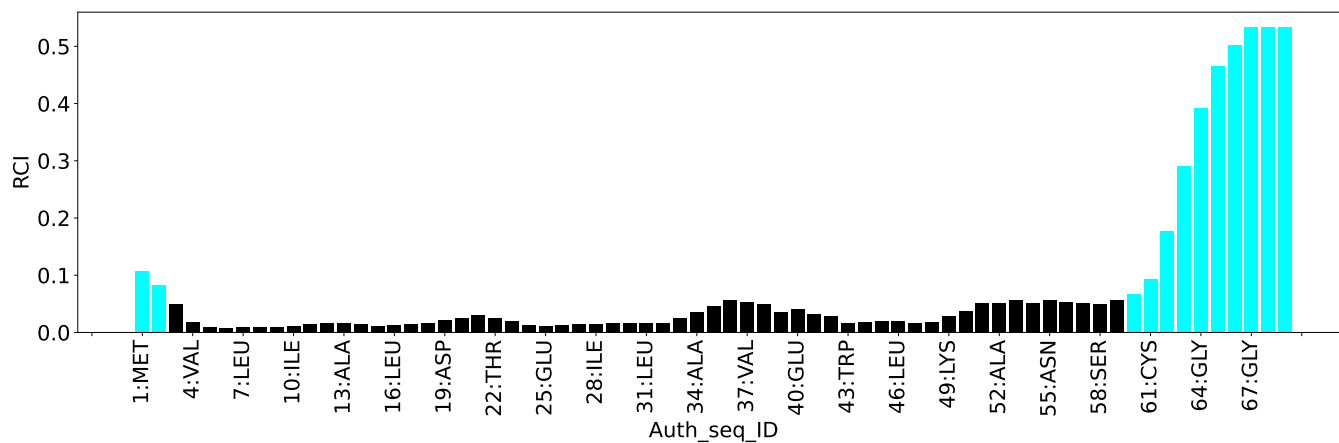
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	6	GLU	HG2	1.04	1.24 – 3.30	-6.0

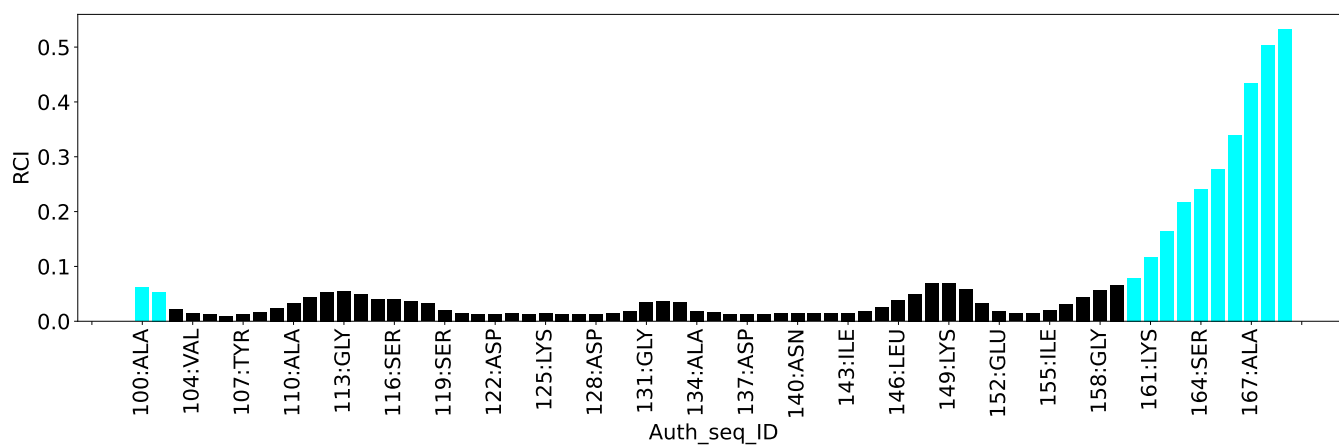
#### 7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



## 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	4675
Intra-residue ( $ i-j =0$ )	2419
Sequential ( $ i-j =1$ )	693
Medium range ( $ i-j >1$ and $ i-j <5$ )	583
Long range ( $ i-j \geq 5$ )	453
Inter-chain	417
Hydrogen bond restraints	110
Disulfide bond restraints	0
Total dihedral-angle restraints	140
Number of unmapped restraints	0
Number of restraints per residue	34.6
Number of long range restraints per residue <sup>1</sup>	3.3

<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)	238.4	0.2
0.2-0.5 (Medium)	347.1	0.5
>0.5 (Large)	275.9	4.33

### 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)	0.9	3.44
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis i

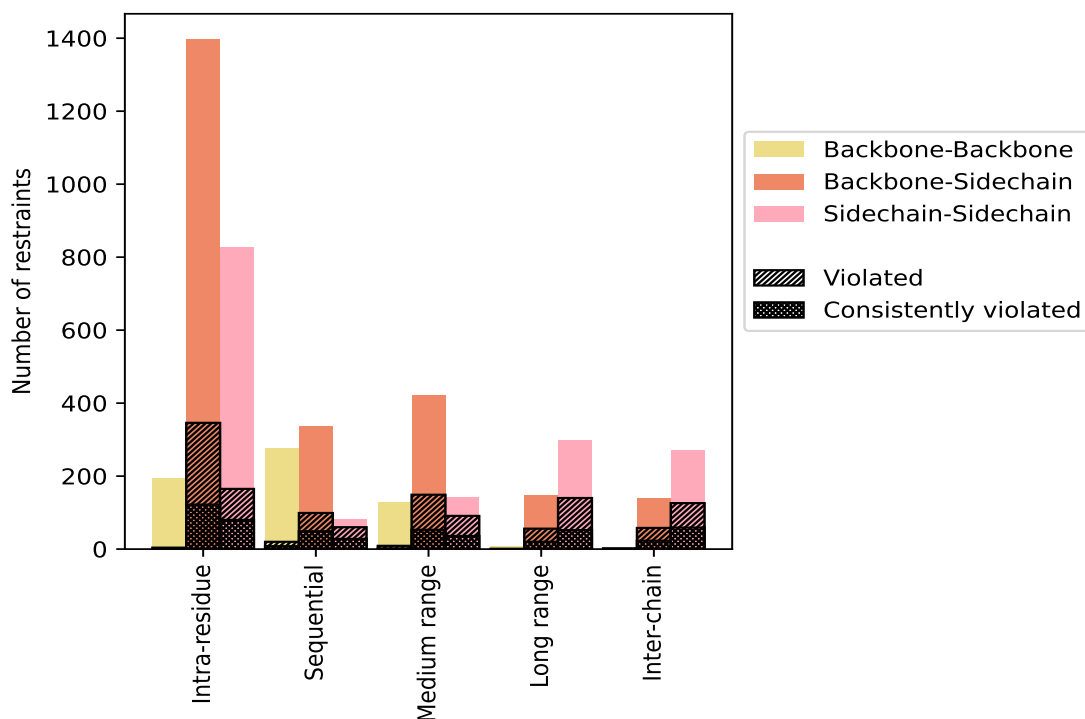
### 9.1 Summary of distance violations i

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

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>2419</b>	<b>51.7</b>	<b>515</b>	<b>21.3</b>	<b>11.0</b>	<b>203</b>	<b>8.4</b>	<b>4.3</b>
Backbone-Backbone	194	4.1	4	2.1	0.1	1	0.5	0.0
Backbone-Sidechain	1397	29.9	346	24.8	7.4	122	8.7	2.6
Sidechain-Sidechain	828	17.7	165	19.9	3.5	80	9.7	1.7
<b>Sequential (<math> i-j =1</math>)</b>	<b>693</b>	<b>14.8</b>	<b>179</b>	<b>25.8</b>	<b>3.8</b>	<b>85</b>	<b>12.3</b>	<b>1.8</b>
Backbone-Backbone	276	5.9	20	7.2	0.4	8	2.9	0.2
Backbone-Sidechain	335	7.2	99	29.6	2.1	49	14.6	1.0
Sidechain-Sidechain	82	1.8	60	73.2	1.3	28	34.1	0.6
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>583</b>	<b>12.5</b>	<b>217</b>	<b>37.2</b>	<b>4.6</b>	<b>82</b>	<b>14.1</b>	<b>1.8</b>
Backbone-Backbone	128	2.7	9	7.0	0.2	2	1.6	0.0
Backbone-Sidechain	312	6.7	117	37.5	2.5	44	14.1	0.9
Sidechain-Sidechain	143	3.1	91	63.6	1.9	36	25.2	0.8
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>453</b>	<b>9.7</b>	<b>197</b>	<b>43.5</b>	<b>4.2</b>	<b>72</b>	<b>15.9</b>	<b>1.5</b>
Backbone-Backbone	8	0.2	1	12.5	0.0	0	0.0	0.0
Backbone-Sidechain	146	3.1	56	38.4	1.2	20	13.7	0.4
Sidechain-Sidechain	299	6.4	140	46.8	3.0	52	17.4	1.1
<b>Inter-chain</b>	<b>417</b>	<b>8.9</b>	<b>186</b>	<b>44.6</b>	<b>4.0</b>	<b>83</b>	<b>19.9</b>	<b>1.8</b>
Backbone-Backbone	6	0.1	2	33.3	0.0	1	16.7	0.0
Backbone-Sidechain	140	3.0	58	41.4	1.2	23	16.4	0.5
Sidechain-Sidechain	271	5.8	126	46.5	2.7	59	21.8	1.3
<b>Hydrogen bond</b>	<b>110</b>	<b>2.4</b>	<b>32</b>	<b>29.1</b>	<b>0.7</b>	<b>9</b>	<b>8.2</b>	<b>0.2</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>4675</b>	<b>100.0</b>	<b>1326</b>	<b>28.4</b>	<b>28.4</b>	<b>534</b>	<b>11.4</b>	<b>11.4</b>
Backbone-Backbone	612	13.1	36	5.9	0.8	12	2.0	0.3
Backbone-Sidechain	2440	52.2	708	29.0	15.1	267	10.9	5.7
Sidechain-Sidechain	1623	34.7	582	35.9	12.4	255	15.7	5.5

<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 disulfid bonds are counted in their appropriate category on the x-axis

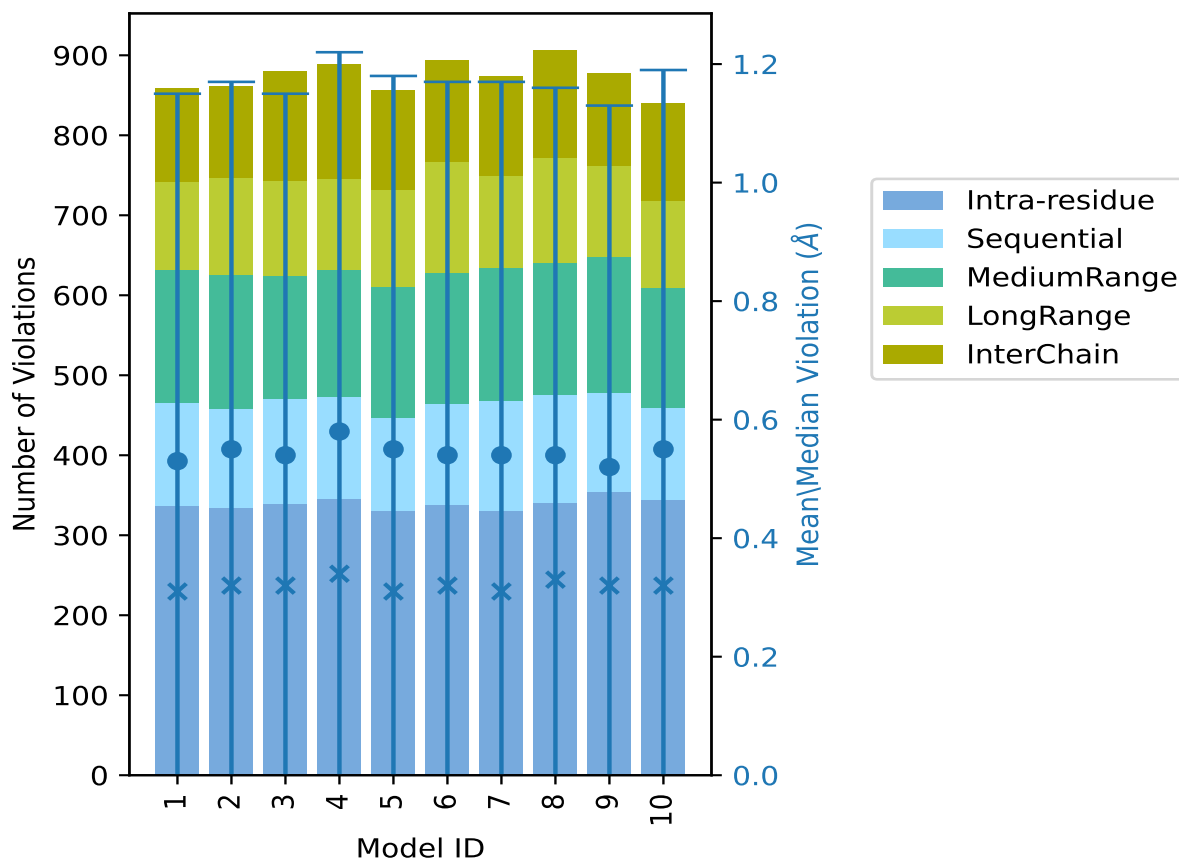
## 9.2 Distance violation statistics for each model [i](#)

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	337	129	166	110	117	859	0.53	4.21	0.62	0.31
2	335	123	168	121	115	862	0.55	4.3	0.62	0.32
3	339	132	154	118	137	880	0.54	4.27	0.61	0.32
4	346	127	158	115	143	889	0.58	4.3	0.64	0.34
5	330	117	163	121	125	856	0.55	4.3	0.63	0.31
6	338	126	164	139	127	894	0.54	4.33	0.63	0.32
7	331	137	166	116	124	874	0.54	4.24	0.63	0.31
8	341	134	166	131	135	907	0.54	4.32	0.62	0.33
9	354	124	170	114	116	878	0.52	4.33	0.61	0.32
10	345	114	150	109	122	840	0.55	4.28	0.64	0.32

<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, 3271(IR:1904, SQ:514, MR:366, LR:256, IC:231) 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>	%
68	20	20	25	25	158	1	10.0
42	14	16	22	20	114	2	20.0
35	7	15	26	14	97	3	30.0

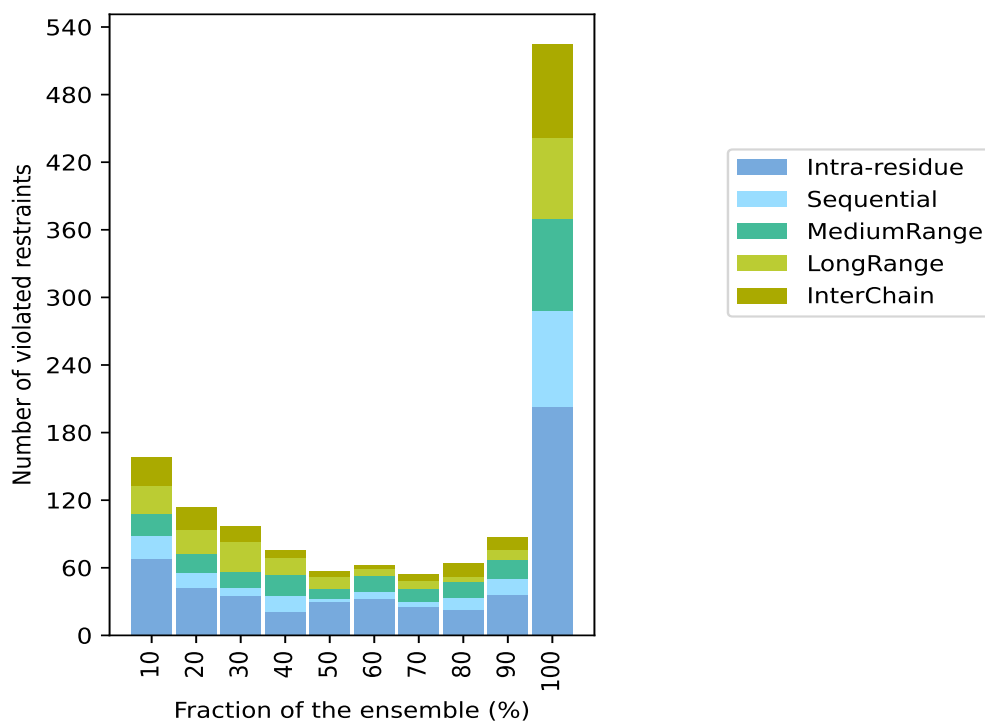
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
21	14	19	15	7	76	4	40.0
30	3	8	11	5	57	5	50.0
32	7	14	6	3	62	6	60.0
25	5	11	7	6	54	7	70.0
23	10	15	4	12	64	8	80.0
36	14	17	9	11	87	9	90.0
203	85	82	72	83	525	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](#)

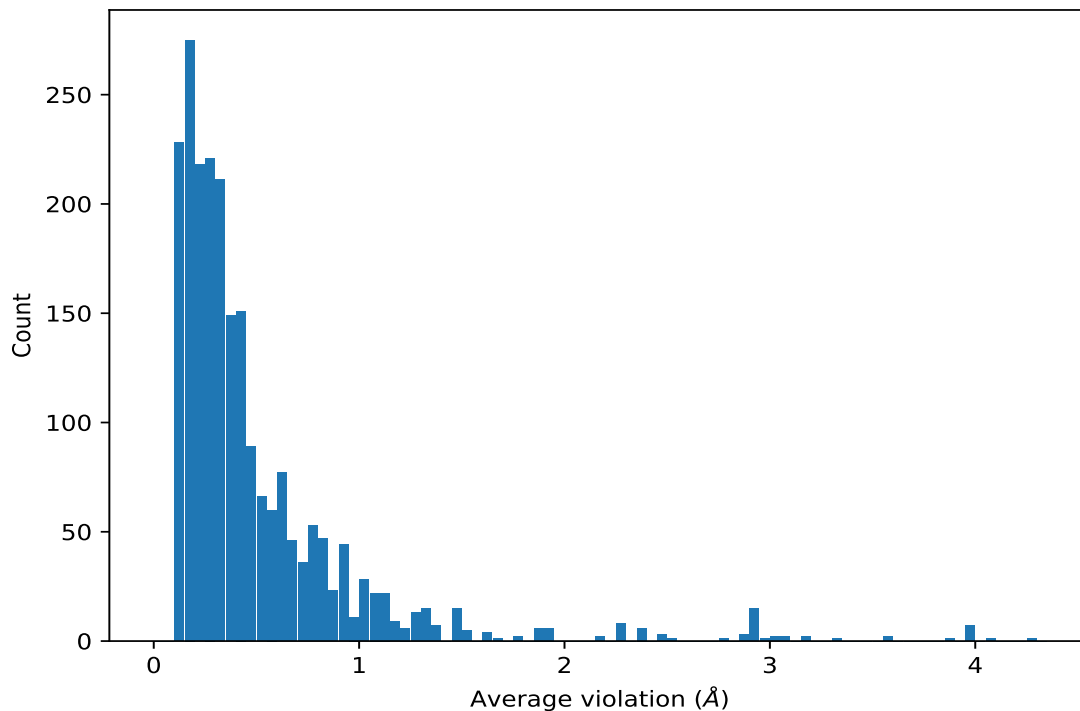


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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)
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	10	4.29	0.04	4.3
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	10	4.08	0.04	4.09
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	10	3.97	0.05	4.0
(2,1215)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	10	3.96	0.08	3.95
(2,1215)	2:159:B:ILE:HG21	1:11:A:TYR:HE2	10	3.96	0.08	3.95
(2,1215)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	10	3.96	0.08	3.95
(2,3505)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	10	3.96	0.08	3.95
(2,3505)	2:159:B:ILE:HG21	1:11:A:TYR:HE2	10	3.96	0.08	3.95
(2,3505)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	10	3.96	0.08	3.95
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	10	3.88	0.05	3.9
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	10	3.59	0.15	3.59
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	10	3.59	0.15	3.59
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	10	3.3	0.05	3.3
(2,869)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	10	3.19	0.17	3.14
(2,869)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	10	3.19	0.17	3.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,3449)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	10	3.05	0.18	3.0
(2,3449)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	10	3.05	0.18	3.0
(2,2740)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	10	3.03	0.17	2.99
(2,2740)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	10	3.03	0.17	2.99
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	2.95	0.1	2.97
(2,978)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	10	2.94	0.19	2.97
(2,978)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	10	2.94	0.19	2.97
(2,978)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	10	2.94	0.19	2.97
(2,2909)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	10	2.94	0.19	2.97
(2,2909)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	10	2.94	0.19	2.97
(2,2909)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	10	2.94	0.19	2.97
(2,977)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	10	2.93	0.12	2.87
(2,977)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	10	2.93	0.12	2.87
(2,977)	2:127:B:LEU:HD21	2:103:B:TYR:HD2	10	2.93	0.12	2.87
(2,2905)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	10	2.93	0.12	2.87
(2,2905)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	10	2.93	0.12	2.87
(2,2905)	2:127:B:LEU:HD21	2:103:B:TYR:HD2	10	2.93	0.12	2.87
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	2.93	0.1	2.95
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	10	2.9	0.09	2.88
(2,799)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	10	2.9	0.09	2.88
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	10	2.86	0.18	2.91
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	10	2.86	0.18	2.91
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	10	2.86	0.18	2.91
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	2.76	0.05	2.78
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	10	2.54	0.09	2.54
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	2.49	0.05	2.5
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	10	2.46	0.09	2.44
(2,3423)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	10	2.46	0.09	2.44
(2,2101)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	10	2.37	0.06	2.38
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	10	2.37	0.06	2.38
(2,396)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	10	2.37	0.07	2.37
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	10	2.37	0.07	2.37
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	10	2.36	0.09	2.34
(2,2656)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	10	2.36	0.09	2.34
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	2.28	0.05	2.3
(2,1027)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	10	2.27	0.19	2.28
(2,1027)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	10	2.27	0.19	2.28
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	10	2.27	0.07	2.26
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD23	10	2.27	0.07	2.26
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	10	2.27	0.07	2.26
(2,2623)	1:11:A:TYR:HD2	1:14:A:LEU:HD22	10	2.27	0.07	2.26
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	2.25	0.1	2.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2975)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	10	2.18	0.19	2.2
(2,2975)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	10	2.18	0.19	2.2
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	1.93	0.1	1.96
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	10	1.91	0.07	1.9
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD23	10	1.91	0.07	1.9
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	10	1.91	0.07	1.9
(2,770)	1:11:A:TYR:HD2	1:14:A:LEU:HD22	10	1.91	0.07	1.9
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	10	1.91	0.06	1.9
(2,3500)	2:159:B:ILE:HD12	1:59:A:LEU:HD11	10	1.89	0.09	1.92
(2,3500)	2:159:B:ILE:HD11	1:59:A:LEU:HD11	10	1.89	0.09	1.92
(2,3500)	2:159:B:ILE:HD11	1:59:A:LEU:HD12	10	1.89	0.09	1.92
(2,3500)	2:159:B:ILE:HD12	1:59:A:LEU:HD12	10	1.89	0.09	1.92
(2,3500)	2:159:B:ILE:HD13	1:59:A:LEU:HD12	10	1.89	0.09	1.92
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	10	1.87	0.08	1.88
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	10	1.79	0.03	1.8
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	10	1.77	0.15	1.8
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	10	1.66	0.07	1.65
(2,3443)	2:110:B:ALA:HB1	1:37:A:VAL:HG13	10	1.62	0.07	1.6
(2,3443)	2:110:B:ALA:HB3	1:37:A:VAL:HG13	10	1.62	0.07	1.6
(2,3443)	2:110:B:ALA:HB1	1:37:A:VAL:HG12	10	1.62	0.07	1.6
(2,3443)	2:110:B:ALA:HB3	1:37:A:VAL:HG12	10	1.62	0.07	1.6
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	10	1.54	0.15	1.56
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	1.52	0.01	1.53
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	10	1.52	0.08	1.54
(2,1182)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	10	1.52	0.08	1.5
(2,1182)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	10	1.52	0.08	1.5
(2,1262)	2:155:B:ILE:HG13	1:7:A:LEU:HD21	10	1.49	0.23	1.47
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	10	1.49	0.23	1.47
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	10	1.49	0.23	1.47
(2,1262)	2:155:B:ILE:HG13	1:7:A:LEU:HD23	10	1.49	0.23	1.47
(2,595)	1:37:A:VAL:HG13	2:114:B:GLY:HA3	10	1.48	0.29	1.56
(2,595)	1:37:A:VAL:HG12	1:39:A:VAL:HA	10	1.48	0.29	1.56
(2,595)	1:37:A:VAL:HG12	2:114:B:GLY:HA3	10	1.48	0.29	1.56
(2,595)	1:37:A:VAL:HG11	1:39:A:VAL:HA	10	1.48	0.29	1.56
(2,3183)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	10	1.47	0.08	1.44
(2,3183)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	10	1.47	0.08	1.44
(2,3395)	1:39:A:VAL:HG21	2:109:B:LEU:HD13	10	1.45	0.07	1.44
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	10	1.45	0.07	1.44
(2,3395)	1:39:A:VAL:HG21	2:109:B:LEU:HD12	10	1.45	0.07	1.44
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD22	10	1.45	0.07	1.44
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	10	1.45	0.07	1.44
(2,1714)	2:121:B:LYS:HD2	2:121:B:LYS:HB3	10	1.38	0.03	1.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	10	1.38	0.03	1.38
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	1.38	0.05	1.4
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	1.36	0.01	1.37
(2,3510)	2:162:B:LEU:HD11	1:56:A:ILE:HG13	10	1.35	0.26	1.42
(2,3510)	2:162:B:LEU:HD12	1:56:A:ILE:HG13	10	1.35	0.26	1.42
(2,3510)	2:162:B:LEU:HD13	1:56:A:ILE:HG13	10	1.35	0.26	1.42
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	10	1.34	0.09	1.34
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	10	1.34	0.17	1.4
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD12	10	1.34	0.17	1.4
(2,841)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	10	1.32	0.19	1.27
(2,841)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	10	1.32	0.19	1.27
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.32	0.02	1.31
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD23	10	1.3	0.42	1.42
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD21	10	1.3	0.42	1.42
(2,1948)	2:154:B:VAL:HG23	2:151:B:ILE:HG13	10	1.3	0.34	1.38
(2,1948)	2:154:B:VAL:HG13	2:155:B:ILE:HG12	10	1.3	0.34	1.38
(2,1948)	2:154:B:VAL:HG23	2:149:B:LYS:HD3	10	1.3	0.34	1.38
(2,1948)	2:154:B:VAL:HG22	2:149:B:LYS:HD2	10	1.3	0.34	1.38
(2,1948)	2:154:B:VAL:HG12	2:155:B:ILE:HG12	10	1.3	0.34	1.38
(2,3486)	2:132:B:ILE:HG22	1:16:A:LEU:HD12	10	1.28	0.13	1.31
(2,3486)	2:132:B:ILE:HG23	1:16:A:LEU:HD13	10	1.28	0.13	1.31
(2,3486)	2:132:B:ILE:HG22	1:16:A:LEU:HD13	10	1.28	0.13	1.31
(2,3486)	2:132:B:ILE:HG21	1:16:A:LEU:HD13	10	1.28	0.13	1.31
(2,3486)	2:132:B:ILE:HG23	1:16:A:LEU:HD11	10	1.28	0.13	1.31
(2,3486)	2:132:B:ILE:HG21	1:16:A:LEU:HD11	10	1.28	0.13	1.31
(2,3486)	2:132:B:ILE:HG22	1:16:A:LEU:HD11	10	1.28	0.13	1.31
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD11	10	1.27	0.26	1.27
(2,513)	1:27:A:LYS:HG3	1:28:A:ILE:HD11	10	1.27	0.26	1.27
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD13	10	1.27	0.26	1.27
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	10	1.26	0.25	1.29
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD3	10	1.26	0.25	1.29
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.24	0.02	1.23
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.2	0.02	1.2
(2,3437)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	10	1.18	0.19	1.14
(2,3437)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	10	1.18	0.19	1.14
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG11	10	1.18	0.1	1.2
(2,186)	2:111:B:ALA:H	2:109:B:LEU:HD11	10	1.18	0.1	1.2
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG13	10	1.18	0.1	1.2
(2,940)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	10	1.14	0.13	1.16
(2,940)	2:123:B:ILE:HG21	2:103:B:TYR:HE2	10	1.14	0.13	1.16
(2,940)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	10	1.14	0.13	1.16
(2,2852)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	10	1.14	0.13	1.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2852)	2:123:B:ILE:HG21	2:103:B:TYR:HE2	10	1.14	0.13	1.16
(2,2852)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	10	1.14	0.13	1.16
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	10	1.14	0.12	1.13
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	10	1.14	0.12	1.13
(2,3513)	2:155:B:ILE:HG23	1:11:A:TYR:HE2	10	1.14	0.15	1.13
(2,3513)	2:155:B:ILE:HG21	1:11:A:TYR:HE2	10	1.14	0.15	1.13
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	10	1.13	0.07	1.12
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	10	1.12	0.12	1.12
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	10	1.12	0.03	1.11
(2,369)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	10	1.12	0.1	1.09
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	10	1.12	0.1	1.09
(2,369)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	1.12	0.1	1.09
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD12	10	1.11	0.04	1.12
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD13	10	1.11	0.04	1.12
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD11	10	1.11	0.04	1.12
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	10	1.08	0.57	1.21
(2,3427)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	10	1.07	0.16	1.13
(2,3427)	2:108:B:LEU:HD21	1:15:A:ILE:HD13	10	1.07	0.16	1.13
(2,3427)	2:108:B:LEU:HD22	1:15:A:ILE:HD11	10	1.07	0.16	1.13
(2,3427)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	10	1.07	0.16	1.13
(2,3427)	2:108:B:LEU:HD22	1:7:A:LEU:HD22	10	1.07	0.16	1.13
(2,3428)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	10	1.07	0.16	1.13
(2,3428)	2:108:B:LEU:HD21	1:15:A:ILE:HD13	10	1.07	0.16	1.13
(2,3428)	2:108:B:LEU:HD22	1:15:A:ILE:HD11	10	1.07	0.16	1.13
(2,3428)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	10	1.07	0.16	1.13
(2,3428)	2:108:B:LEU:HD22	1:7:A:LEU:HD22	10	1.07	0.16	1.13
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	10	1.07	0.14	1.06
(2,2729)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	10	1.06	0.09	1.06
(2,2729)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	10	1.06	0.09	1.06
(2,2729)	2:111:B:ALA:HB2	2:151:B:ILE:HD12	10	1.06	0.09	1.06
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	10	1.06	0.79	1.0
(2,794)	2:104:B:VAL:HG21	2:105:B:ALA:HA	10	1.06	0.79	1.0
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.05	0.02	1.05
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	10	1.05	0.04	1.04
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	10	1.04	0.32	1.18
(2,1486)	1:39:A:VAL:HG13	1:5:A:SER:HA	10	1.03	0.06	1.04
(2,1486)	1:39:A:VAL:HG11	1:5:A:SER:HA	10	1.03	0.06	1.04
(2,1486)	1:39:A:VAL:HG22	1:5:A:SER:HA	10	1.03	0.06	1.04
(2,1486)	1:39:A:VAL:HG12	1:5:A:SER:HA	10	1.03	0.06	1.04
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG13	10	1.03	0.36	0.88
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG12	10	1.03	0.36	0.88
(2,3456)	1:15:A:ILE:HD12	2:126:B:ILE:HD12	10	1.03	0.36	0.88

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,3456)	2:126:B:ILE:HD12	1:37:A:VAL:HG12	10	1.03	0.36	0.88
(2,3456)	1:15:A:ILE:HD11	2:126:B:ILE:HD12	10	1.03	0.36	0.88
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	10	1.01	0.57	1.14
(2,3410)	1:60:A:ILE:HD13	2:159:B:ILE:HG23	10	1.0	0.62	1.45
(2,3410)	1:60:A:ILE:HD12	2:159:B:ILE:HG21	10	1.0	0.62	1.45
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	10	1.0	0.32	1.15
(2,855)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	10	1.0	0.09	1.0
(2,855)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	10	1.0	0.09	1.0
(2,855)	2:111:B:ALA:HB2	2:151:B:ILE:HD12	10	1.0	0.09	1.0
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	10	1.0	0.12	1.0
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	10	0.97	0.07	0.96
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	10	0.96	0.26	1.08
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	10	0.95	0.08	0.96
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	10	0.95	0.02	0.94
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	10	0.94	0.07	0.94
(2,3351)	1:16:A:LEU:HD13	2:130:B:VAL:HA	10	0.93	0.06	0.92
(2,3351)	1:16:A:LEU:HD11	2:130:B:VAL:HA	10	0.93	0.06	0.92
(2,3351)	1:16:A:LEU:HD12	2:130:B:VAL:HA	10	0.93	0.06	0.92
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB2	10	0.92	0.16	0.88
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB3	10	0.92	0.16	0.88
(2,3177)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	10	0.92	0.26	0.94
(2,3177)	2:154:B:VAL:HG11	2:146:B:LEU:HD21	10	0.92	0.26	0.94
(2,3177)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	10	0.92	0.26	0.94
(2,3177)	2:154:B:VAL:HG12	2:146:B:LEU:HD11	10	0.92	0.26	0.94
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	10	0.92	0.04	0.92
(2,2181)	1:17:A:HIS:HB2	1:56:A:ILE:HG23	10	0.91	0.16	0.83
(2,2181)	1:17:A:HIS:HB3	1:56:A:ILE:HG23	10	0.91	0.16	0.83
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.91	0.15	0.97
(2,619)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	10	0.91	0.15	0.97
(2,3502)	2:159:B:ILE:HD11	1:60:A:ILE:HG13	10	0.91	0.18	0.96
(2,3502)	2:159:B:ILE:HD12	1:60:A:ILE:HG13	10	0.91	0.18	0.96
(2,3173)	2:154:B:VAL:HG23	2:151:B:ILE:HG12	10	0.89	0.11	0.88
(2,3173)	2:154:B:VAL:HG21	2:151:B:ILE:HG12	10	0.89	0.11	0.88
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	10	0.89	0.24	0.98
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	10	0.88	0.18	0.82
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.88	0.19	0.8
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	10	0.87	0.11	0.84
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	10	0.87	0.36	1.04
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	10	0.87	0.1	0.84
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	10	0.87	0.1	0.84
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.86	0.0	0.86
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	10	0.86	0.01	0.86

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	10	0.85	0.17	0.92
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD12	10	0.85	0.17	0.92
(2,2069)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	10	0.84	0.1	0.82
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	10	0.84	0.1	0.82
(2,2069)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	0.84	0.1	0.82
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	10	0.84	0.08	0.86
(2,1542)	1:51:A:LEU:HD22	1:56:A:ILE:HB	10	0.84	0.7	0.65
(2,1542)	1:51:A:LEU:HD23	1:56:A:ILE:HB	10	0.84	0.7	0.65
(2,1542)	1:51:A:LEU:HD21	1:56:A:ILE:HB	10	0.84	0.7	0.65
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD11	10	0.83	0.86	0.57
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD13	10	0.83	0.86	0.57
(2,2462)	1:47:A:PHE:HB2	1:59:A:LEU:HD13	10	0.83	0.86	0.57
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD12	10	0.83	0.86	0.57
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.83	0.15	0.89
(2,2412)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	10	0.83	0.15	0.89
(2,386)	1:10:A:ILE:HD11	1:47:A:PHE:HE2	10	0.82	0.15	0.84
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE2	10	0.82	0.15	0.84
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE1	10	0.82	0.15	0.84
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB3	10	0.82	0.18	0.79
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB2	10	0.82	0.18	0.79
(2,3191)	2:156:B:ALA:HB3	2:153:B:ASP:HB2	10	0.82	0.18	0.79
(2,3191)	2:156:B:ALA:HB2	2:153:B:ASP:HB2	10	0.82	0.18	0.79
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	10	0.82	0.02	0.82
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	10	0.82	0.09	0.82
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.81	0.0	0.81
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	10	0.81	0.08	0.84
(2,3496)	2:156:B:ALA:HB1	1:7:A:LEU:HB2	10	0.81	0.08	0.84
(2,3496)	2:156:B:ALA:HB3	1:7:A:LEU:HB2	10	0.81	0.08	0.84
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG11	10	0.81	0.03	0.8
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG12	10	0.81	0.03	0.8
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG13	10	0.81	0.03	0.8
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	10	0.81	0.12	0.88
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE1	10	0.81	0.12	0.88
(2,370)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	10	0.81	0.1	0.78
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	10	0.81	0.1	0.78
(2,370)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	0.81	0.1	0.78
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	10	0.8	0.05	0.82
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	10	0.79	0.32	0.94
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG12	10	0.78	0.18	0.84
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG22	10	0.78	0.18	0.84
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG23	10	0.78	0.18	0.84
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG11	10	0.78	0.18	0.84

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	10	0.78	0.3	0.88
(2,3503)	1:59:A:LEU:HD11	2:159:B:ILE:HG12	10	0.78	0.11	0.82
(2,3503)	1:59:A:LEU:HD11	2:159:B:ILE:HG13	10	0.78	0.11	0.82
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG13	10	0.78	0.11	0.82
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	10	0.78	0.11	0.82
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.77	0.19	0.7
(2,2721)	2:110:B:ALA:HB2	2:119:B:SER:H	10	0.77	0.07	0.76
(2,2721)	2:110:B:ALA:HB1	2:119:B:SER:H	10	0.77	0.07	0.76
(2,1173)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	10	0.76	0.26	0.78
(2,1173)	2:154:B:VAL:HG11	2:146:B:LEU:HD21	10	0.76	0.26	0.78
(2,1173)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	10	0.76	0.26	0.78
(2,1173)	2:154:B:VAL:HG12	2:146:B:LEU:HD11	10	0.76	0.26	0.78
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	10	0.76	0.05	0.76
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG21	10	0.76	0.05	0.76
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.76	0.15	0.82
(2,1491)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	10	0.76	0.15	0.82
(2,856)	2:111:B:ALA:HB1	2:107:B:TYR:HE1	10	0.76	0.06	0.77
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	10	0.76	0.06	0.77
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	10	0.76	0.06	0.77
(2,856)	2:111:B:ALA:HB2	2:107:B:TYR:HD1	10	0.76	0.06	0.77
(2,856)	2:111:B:ALA:HB2	2:107:B:TYR:HE1	10	0.76	0.06	0.77
(2,1329)	1:14:A:LEU:HA	1:56:A:ILE:HG23	10	0.76	0.04	0.76
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB2	10	0.76	0.04	0.76
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB1	10	0.76	0.04	0.76
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB3	10	0.76	0.04	0.76
(2,1658)	2:111:B:ALA:HB3	2:151:B:ILE:HG13	10	0.76	0.12	0.77
(2,1658)	2:111:B:ALA:HB2	2:151:B:ILE:HG13	10	0.76	0.12	0.77
(2,1658)	2:111:B:ALA:HB1	2:151:B:ILE:HG13	10	0.76	0.12	0.77
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.74	0.19	0.67
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.74	0.19	0.66
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	10	0.72	0.12	0.7
(2,1063)	2:139:B:LEU:HD21	2:103:B:TYR:HE1	10	0.71	0.55	0.7
(2,1063)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	10	0.71	0.55	0.7
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD13	10	0.7	0.12	0.74
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD12	10	0.7	0.12	0.74
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	10	0.7	0.09	0.7
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD23	10	0.7	0.04	0.7
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD22	10	0.7	0.04	0.7
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD21	10	0.7	0.04	0.7
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG22	10	0.69	0.12	0.78
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG21	10	0.69	0.12	0.78
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG23	10	0.69	0.12	0.78

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD23	10	0.69	0.01	0.69
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	10	0.69	0.01	0.69
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD22	10	0.69	0.01	0.69
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD21	10	0.69	0.01	0.69
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	10	0.69	0.24	0.81
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	10	0.68	0.25	0.81
(2,2810)	2:119:B:SER:HB2	2:120:B:ALA:HB1	10	0.68	0.06	0.68
(2,2810)	2:119:B:SER:HB3	2:120:B:ALA:HB1	10	0.68	0.06	0.68
(2,2810)	2:119:B:SER:HB3	2:120:B:ALA:HB2	10	0.68	0.06	0.68
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	10	0.68	0.01	0.68
(2,2725)	2:111:B:ALA:HB1	2:107:B:TYR:HE1	10	0.67	0.06	0.68
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	10	0.67	0.06	0.68
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	10	0.67	0.06	0.68
(2,2725)	2:111:B:ALA:HB2	2:107:B:TYR:HD1	10	0.67	0.06	0.68
(2,2725)	2:111:B:ALA:HB2	2:107:B:TYR:HE1	10	0.67	0.06	0.68
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	10	0.67	0.53	0.38
(2,951)	2:125:B:LYS:HD3	2:129:B:SER:HB3	10	0.67	0.53	0.38
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD22	10	0.67	0.1	0.66
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD23	10	0.67	0.1	0.66
(2,2685)	2:105:B:ALA:HB2	2:108:B:LEU:HD22	10	0.67	0.1	0.66
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	10	0.66	0.04	0.68
(2,206)	2:115:B:ASN:H	2:112:B:LEU:H	10	0.66	0.04	0.68
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.66	0.0	0.66
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	10	0.65	0.39	0.62
(2,3195)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	10	0.65	0.39	0.62
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	10	0.64	0.39	0.61
(2,1186)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	10	0.64	0.39	0.61
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	10	0.64	0.2	0.64
(2,498)	1:25:A:GLU:HG3	1:48:A:ALA:HB3	10	0.64	0.2	0.64
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB3	10	0.64	0.2	0.64
(2,498)	1:25:A:GLU:HG3	1:48:A:ALA:HB1	10	0.64	0.2	0.64
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	10	0.64	0.16	0.7
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.63	0.01	0.64
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.63	0.19	0.55
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	10	0.62	0.08	0.64
(2,1172)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	10	0.62	0.03	0.61
(2,1172)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	10	0.62	0.03	0.61
(2,3171)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	10	0.62	0.03	0.61
(2,3171)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	10	0.62	0.03	0.61
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	0.61	0.02	0.61
(2,3515)	2:155:B:ILE:HG13	1:7:A:LEU:HD21	10	0.61	0.23	0.59
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	10	0.61	0.23	0.59

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	10	0.61	0.23	0.59
(2,3515)	2:155:B:ILE:HG13	1:7:A:LEU:HD23	10	0.61	0.23	0.59
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	10	0.61	0.01	0.61
(2,3151)	2:152:B:GLU:HB2	2:151:B:ILE:HG22	10	0.61	0.22	0.6
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	10	0.61	0.22	0.6
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG23	10	0.61	0.22	0.6
(2,3179)	2:154:B:VAL:HG13	2:155:B:ILE:H	10	0.61	0.06	0.62
(2,3179)	2:154:B:VAL:HG12	2:155:B:ILE:H	10	0.61	0.06	0.62
(2,3179)	2:154:B:VAL:HG11	2:155:B:ILE:H	10	0.61	0.06	0.62
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.6	0.01	0.6
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	10	0.6	0.05	0.62
(2,2095)	1:10:A:ILE:HD11	1:47:A:PHE:HE2	10	0.6	0.02	0.59
(2,2095)	1:10:A:ILE:HD11	1:9:A:CYS:H	10	0.6	0.02	0.59
(2,2095)	1:10:A:ILE:HD12	1:9:A:CYS:H	10	0.6	0.02	0.59
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB3	10	0.59	0.03	0.58
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB2	10	0.59	0.03	0.58
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB1	10	0.59	0.03	0.58
(2,1285)	1:4:A:VAL:HG23	1:7:A:LEU:HB3	10	0.59	0.05	0.6
(2,1285)	1:4:A:VAL:HG22	1:7:A:LEU:HB3	10	0.59	0.05	0.6
(2,1285)	1:4:A:VAL:HG21	1:7:A:LEU:HB3	10	0.59	0.05	0.6
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	10	0.58	0.08	0.58
(2,695)	1:51:A:LEU:HD11	1:48:A:ALA:HA	10	0.58	0.95	0.28
(2,695)	1:51:A:LEU:HD13	1:48:A:ALA:HA	10	0.58	0.95	0.28
(2,695)	1:51:A:LEU:HD12	1:48:A:ALA:HA	10	0.58	0.95	0.28
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB2	10	0.58	0.24	0.59
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB1	10	0.58	0.24	0.59
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB3	10	0.58	0.24	0.59
(2,3322)	1:10:A:ILE:HD11	2:159:B:ILE:HG22	10	0.57	0.52	0.26
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG21	10	0.57	0.52	0.26
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG22	10	0.57	0.52	0.26
(2,850)	2:110:B:ALA:HB2	2:118:B:PRO:HA	10	0.57	0.08	0.57
(2,850)	2:110:B:ALA:HB1	2:118:B:PRO:HA	10	0.57	0.08	0.57
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	10	0.57	0.05	0.58
(2,2166)	1:16:A:LEU:HD21	1:27:A:LYS:HE3	10	0.57	0.2	0.57
(2,2166)	1:16:A:LEU:HD11	1:27:A:LYS:HE3	10	0.57	0.2	0.57
(2,2166)	1:16:A:LEU:HD23	1:27:A:LYS:HE3	10	0.57	0.2	0.57
(2,2166)	1:16:A:LEU:HD11	1:27:A:LYS:HE2	10	0.57	0.2	0.57
(2,2166)	1:16:A:LEU:HD12	1:27:A:LYS:HE3	10	0.57	0.2	0.57
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.56	0.01	0.56
(2,2716)	2:110:B:ALA:HB2	2:118:B:PRO:HA	10	0.56	0.08	0.56
(2,2716)	2:110:B:ALA:HB1	2:118:B:PRO:HA	10	0.56	0.08	0.56
(2,3464)	2:129:B:SER:HA	1:34:A:ALA:HA	10	0.56	0.21	0.64

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,3464)	2:129:B:SER:HA	1:30:A:ALA:HA	10	0.56	0.21	0.64
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	10	0.55	0.01	0.56
(2,2071)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	10	0.55	0.1	0.52
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	10	0.55	0.1	0.52
(2,2071)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	0.55	0.1	0.52
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	10	0.55	0.08	0.56
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD11	10	0.55	0.08	0.58
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD13	10	0.55	0.08	0.58
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD12	10	0.55	0.08	0.58
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	10	0.55	0.08	0.55
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	10	0.54	0.04	0.55
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	10	0.54	0.17	0.6
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	10	0.54	0.17	0.6
(2,2746)	2:112:B:LEU:HD22	1:7:A:LEU:HG	10	0.54	0.08	0.5
(2,2746)	2:112:B:LEU:HD21	1:7:A:LEU:HG	10	0.54	0.08	0.5
(2,2746)	2:112:B:LEU:HD23	1:7:A:LEU:HG	10	0.54	0.08	0.5
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	10	0.53	0.05	0.56
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	0.53	0.02	0.53
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.53	0.01	0.52
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	10	0.53	0.05	0.56
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	10	0.52	0.02	0.52
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD11	10	0.52	0.35	0.44
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD13	10	0.52	0.35	0.44
(2,1520)	1:47:A:PHE:HA	1:46:A:LEU:HD13	10	0.52	0.35	0.44
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD12	10	0.52	0.35	0.44
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD12	10	0.51	0.18	0.52
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD21	10	0.51	0.18	0.52
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD22	10	0.51	0.18	0.52
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD23	10	0.51	0.18	0.52
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	10	0.51	0.02	0.52
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.51	0.02	0.52
(2,2703)	2:109:B:LEU:HD12	2:109:B:LEU:H	10	0.51	0.3	0.44
(2,2703)	2:109:B:LEU:HD13	2:109:B:LEU:H	10	0.51	0.3	0.44
(2,2703)	2:109:B:LEU:HD21	2:109:B:LEU:H	10	0.51	0.3	0.44
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD22	10	0.51	0.02	0.5
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD23	10	0.51	0.02	0.5
(2,2581)	1:61:A:CYS:HB3	1:60:A:ILE:H	10	0.51	0.07	0.5
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	10	0.51	0.07	0.5
(2,2072)	1:7:A:LEU:HD11	1:7:A:LEU:H	10	0.51	0.04	0.5
(2,2072)	1:7:A:LEU:HD12	1:7:A:LEU:H	10	0.51	0.04	0.5
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	10	0.51	0.05	0.54
(2,1391)	1:24:A:THR:HG22	1:27:A:LYS:HE3	10	0.5	0.5	0.35

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1391)	1:24:A:THR:HG21	1:27:A:LYS:HE3	10	0.5	0.5	0.35
(2,1391)	1:24:A:THR:HG23	1:27:A:LYS:HE3	10	0.5	0.5	0.35
(2,2722)	2:110:B:ALA:HB1	2:109:B:LEU:HB3	10	0.5	0.08	0.5
(2,2722)	2:110:B:ALA:HB3	2:109:B:LEU:HB3	10	0.5	0.08	0.5
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB2	10	0.5	0.31	0.46
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB3	10	0.5	0.31	0.46
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.5	0.01	0.5
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	10	0.49	0.05	0.48
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	10	0.49	0.05	0.48
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	10	0.49	0.04	0.5
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD1	10	0.49	0.04	0.5
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB2	10	0.48	0.09	0.48
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB1	10	0.48	0.09	0.48
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB3	10	0.48	0.09	0.48
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	10	0.48	0.02	0.49
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	0.48	0.01	0.48
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	10	0.48	0.02	0.48
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG22	10	0.48	0.02	0.48
(2,3361)	1:31:A:LEU:HD11	2:129:B:SER:HA	10	0.47	0.1	0.51
(2,3361)	1:31:A:LEU:HD13	2:129:B:SER:HA	10	0.47	0.1	0.51
(2,3361)	1:31:A:LEU:HD12	2:129:B:SER:HA	10	0.47	0.1	0.51
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	10	0.47	0.01	0.47
(2,1341)	1:15:A:ILE:HD13	1:15:A:ILE:HB	10	0.47	0.04	0.48
(2,1341)	1:15:A:ILE:HD11	1:15:A:ILE:HB	10	0.47	0.04	0.48
(2,1341)	1:15:A:ILE:HD12	1:15:A:ILE:HB	10	0.47	0.04	0.48
(2,3305)	1:4:A:VAL:HG23	2:112:B:LEU:HA	10	0.47	0.13	0.46
(2,3305)	1:4:A:VAL:HG22	2:112:B:LEU:HA	10	0.47	0.13	0.46
(2,3305)	1:4:A:VAL:HG11	2:112:B:LEU:HA	10	0.47	0.13	0.46
(2,2826)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	10	0.47	0.05	0.45
(2,2826)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	10	0.47	0.05	0.45
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	10	0.47	0.03	0.48
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	0.46	0.01	0.46
(2,1659)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	10	0.46	0.09	0.46
(2,1659)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	10	0.46	0.09	0.46
(2,1659)	2:111:B:ALA:HB2	2:151:B:ILE:HD12	10	0.46	0.09	0.46
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	10	0.46	0.03	0.46
(2,3492)	2:152:B:GLU:HG2	1:7:A:LEU:HB3	10	0.46	0.16	0.44
(2,3492)	2:152:B:GLU:HG3	1:7:A:LEU:HB3	10	0.46	0.16	0.44
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.46	0.02	0.46
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	10	0.45	0.05	0.46
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	10	0.45	0.01	0.46
(2,1283)	1:4:A:VAL:HG23	1:7:A:LEU:HD22	10	0.45	0.06	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1283)	1:4:A:VAL:HG22	1:7:A:LEU:HD21	10	0.45	0.06	0.44
(2,1283)	1:4:A:VAL:HG21	1:7:A:LEU:HD21	10	0.45	0.06	0.44
(2,1283)	1:4:A:VAL:HG23	1:7:A:LEU:HD21	10	0.45	0.06	0.44
(2,1283)	1:4:A:VAL:HG21	1:7:A:LEU:HD23	10	0.45	0.06	0.44
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	10	0.45	0.03	0.46
(2,2030)	2:167:B:ALA:HB1	2:167:B:ALA:HA	10	0.45	0.02	0.46
(2,2030)	2:167:B:ALA:HB3	2:167:B:ALA:HA	10	0.45	0.02	0.46
(2,2030)	2:167:B:ALA:HB2	2:167:B:ALA:HA	10	0.45	0.02	0.46
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.44	0.02	0.44
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.44	0.15	0.5
(2,628)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	10	0.44	0.15	0.5
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG22	10	0.44	0.05	0.45
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	10	0.44	0.05	0.45
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	10	0.44	0.13	0.42
(2,3172)	2:154:B:VAL:HG13	2:155:B:ILE:H	10	0.44	0.06	0.45
(2,3172)	2:154:B:VAL:HG12	2:155:B:ILE:H	10	0.44	0.06	0.45
(2,3172)	2:154:B:VAL:HG11	2:155:B:ILE:H	10	0.44	0.06	0.45
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	10	0.44	0.04	0.43
(2,1701)	2:120:B:ALA:HB2	2:139:B:LEU:HB2	10	0.44	0.04	0.43
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	10	0.44	0.03	0.43
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG11	10	0.44	0.02	0.44
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG13	10	0.44	0.02	0.44
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG22	10	0.44	0.02	0.44
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG12	10	0.44	0.02	0.44
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	10	0.43	0.02	0.44
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD2	10	0.43	0.02	0.44
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	10	0.43	0.01	0.43
(2,430)	1:15:A:ILE:HG22	2:106:B:SER:HA	10	0.43	0.04	0.44
(2,430)	1:15:A:ILE:HG23	2:106:B:SER:HA	10	0.43	0.04	0.44
(2,3123)	2:147:B:ASN:HB3	2:148:B:GLY:H	10	0.43	0.07	0.43
(2,3123)	2:147:B:ASN:HB2	2:148:B:GLY:H	10	0.43	0.07	0.43
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	10	0.43	0.18	0.38
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	10	0.43	0.07	0.45
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	10	0.43	0.22	0.28
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	10	0.43	0.08	0.44
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB2	10	0.43	0.08	0.44
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG11	10	0.43	0.07	0.42
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	10	0.43	0.07	0.42
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD13	10	0.43	0.12	0.46
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD12	10	0.43	0.12	0.46
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG23	10	0.43	0.03	0.44
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG22	10	0.43	0.03	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG21	10	0.43	0.03	0.44
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.42	0.01	0.42
(2,1614)	2:101:B:MET:HE2	1:14:A:LEU:HB2	10	0.42	0.14	0.41
(2,1614)	2:101:B:MET:HE1	1:14:A:LEU:HB2	10	0.42	0.14	0.41
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	10	0.42	0.03	0.41
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB2	10	0.42	0.31	0.38
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB3	10	0.42	0.31	0.38
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	10	0.42	0.42	0.24
(2,2742)	1:37:A:VAL:HG22	2:112:B:LEU:HD23	10	0.42	0.42	0.24
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	10	0.42	0.42	0.24
(2,2742)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	10	0.42	0.42	0.24
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD21	10	0.42	0.42	0.24
(2,2742)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	10	0.42	0.42	0.24
(2,2742)	1:37:A:VAL:HG23	2:112:B:LEU:HD21	10	0.42	0.42	0.24
(2,2742)	2:112:B:LEU:HD22	2:109:B:LEU:HD12	10	0.42	0.42	0.24
(2,2612)	1:42:A:PHE:HD1	1:42:A:PHE:HZ	10	0.42	0.0	0.42
(2,2612)	1:42:A:PHE:HD2	1:42:A:PHE:HZ	10	0.42	0.0	0.42
(2,2094)	1:10:A:ILE:HD13	1:7:A:LEU:H	10	0.42	0.05	0.4
(2,2094)	1:10:A:ILE:HD11	1:7:A:LEU:H	10	0.42	0.05	0.4
(2,2368)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	10	0.42	0.37	0.24
(2,2368)	1:37:A:VAL:HG13	2:113:B:GLY:HA2	10	0.42	0.37	0.24
(2,2368)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	10	0.42	0.37	0.24
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG13	10	0.41	0.19	0.35
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG12	10	0.41	0.19	0.35
(2,2715)	2:110:B:ALA:HB2	2:115:B:ASN:H	10	0.41	0.12	0.41
(2,2715)	2:110:B:ALA:HB1	2:115:B:ASN:H	10	0.41	0.12	0.41
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	10	0.41	0.01	0.41
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	10	0.41	0.05	0.43
(2,596)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	10	0.4	0.37	0.23
(2,596)	1:37:A:VAL:HG13	2:113:B:GLY:HA2	10	0.4	0.37	0.23
(2,596)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	10	0.4	0.37	0.23
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD13	10	0.4	0.06	0.42
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD23	10	0.4	0.06	0.42
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD11	10	0.4	0.06	0.42
(2,842)	2:109:B:LEU:HD22	1:12:A:SER:HA	10	0.4	0.54	0.22
(2,842)	2:109:B:LEU:HD23	1:12:A:SER:HA	10	0.4	0.54	0.22
(2,842)	2:109:B:LEU:HD21	1:12:A:SER:HA	10	0.4	0.54	0.22
(2,493)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	10	0.4	0.14	0.36
(2,493)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	10	0.4	0.14	0.36
(2,493)	1:25:A:GLU:HB3	1:48:A:ALA:HB1	10	0.4	0.14	0.36
(2,1992)	2:161:B:LYS:HE2	2:161:B:LYS:HD3	10	0.39	0.04	0.4
(2,1992)	2:161:B:LYS:HE3	2:161:B:LYS:HD2	10	0.39	0.04	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG2	10	0.39	0.15	0.47
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	10	0.39	0.15	0.47
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	10	0.39	0.04	0.4
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG11	10	0.39	0.04	0.4
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG13	10	0.39	0.04	0.4
(2,2709)	2:109:B:LEU:HD22	1:12:A:SER:HA	10	0.39	0.54	0.21
(2,2709)	2:109:B:LEU:HD23	1:12:A:SER:HA	10	0.39	0.54	0.21
(2,2709)	2:109:B:LEU:HD21	1:12:A:SER:HA	10	0.39	0.54	0.21
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD13	10	0.39	0.05	0.38
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD11	10	0.39	0.05	0.38
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD12	10	0.39	0.05	0.38
(2,2456)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	10	0.39	0.03	0.38
(2,2456)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	10	0.39	0.03	0.38
(2,2456)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	10	0.39	0.03	0.38
(2,2004)	2:163:B:ALA:HB3	2:163:B:ALA:HA	10	0.38	0.03	0.38
(2,2004)	2:163:B:ALA:HB1	2:163:B:ALA:HA	10	0.38	0.03	0.38
(2,2004)	2:163:B:ALA:HB2	2:163:B:ALA:HA	10	0.38	0.03	0.38
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	10	0.38	0.03	0.39
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB3	10	0.38	0.03	0.39
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB1	10	0.38	0.03	0.39
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	10	0.38	0.15	0.44
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG23	10	0.38	0.09	0.36
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG22	10	0.38	0.09	0.36
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG21	10	0.38	0.09	0.36
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	10	0.38	0.02	0.38
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.38	0.02	0.38
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG12	10	0.38	0.02	0.38
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG13	10	0.38	0.02	0.38
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	10	0.38	0.11	0.38
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB3	10	0.38	0.11	0.38
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB2	10	0.38	0.11	0.38
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	10	0.37	0.02	0.37
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD21	10	0.37	0.07	0.4
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD23	10	0.37	0.07	0.4
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD22	10	0.37	0.07	0.4
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG23	10	0.37	0.31	0.17
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG13	10	0.37	0.31	0.17
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG22	10	0.37	0.31	0.17
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG11	10	0.37	0.31	0.17
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB3	10	0.37	0.04	0.38
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB2	10	0.37	0.04	0.38
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB1	10	0.37	0.04	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG2	10	0.37	0.1	0.36
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG3	10	0.37	0.1	0.36
(2,1629)	2:105:B:ALA:HB2	2:101:B:MET:HG2	10	0.37	0.1	0.36
(2,1629)	2:105:B:ALA:HB2	2:101:B:MET:HG3	10	0.37	0.1	0.36
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	10	0.36	0.04	0.37
(2,2982)	2:134:B:ALA:HB1	2:124:B:LYS:HA	10	0.36	0.1	0.34
(2,2982)	2:134:B:ALA:HB3	2:124:B:LYS:HA	10	0.36	0.1	0.34
(2,1028)	2:134:B:ALA:HB1	2:124:B:LYS:HA	10	0.36	0.1	0.34
(2,1028)	2:134:B:ALA:HB3	2:124:B:LYS:HA	10	0.36	0.1	0.34
(2,739)	1:59:A:LEU:HD12	1:56:A:ILE:HA	10	0.36	0.09	0.36
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	10	0.36	0.09	0.36
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	10	0.36	0.04	0.36
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB2	10	0.36	0.04	0.36
(2,2100)	1:10:A:ILE:HG23	1:47:A:PHE:HE2	10	0.36	0.08	0.36
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	10	0.36	0.08	0.36
(2,3054)	2:142:B:VAL:HG13	2:107:B:TYR:HD2	10	0.36	0.07	0.34
(2,3054)	2:142:B:VAL:HG11	2:107:B:TYR:HD2	10	0.36	0.07	0.34
(2,3054)	2:142:B:VAL:HG12	2:107:B:TYR:HD2	10	0.36	0.07	0.34
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.36	0.01	0.36
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG12	10	0.36	0.01	0.36
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG13	10	0.36	0.01	0.36
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	10	0.35	0.1	0.36
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB3	10	0.35	0.1	0.36
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	10	0.35	0.1	0.36
(2,1387)	1:23:A:VAL:HG11	1:48:A:ALA:HB1	10	0.35	0.1	0.36
(2,1387)	1:23:A:VAL:HG11	1:48:A:ALA:HB2	10	0.35	0.1	0.36
(2,1387)	1:23:A:VAL:HG13	1:48:A:ALA:HB2	10	0.35	0.1	0.36
(2,3399)	1:59:A:LEU:HD11	2:159:B:ILE:HA	10	0.35	0.04	0.36
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	10	0.35	0.04	0.36
(2,3402)	1:59:A:LEU:HD11	2:159:B:ILE:HA	10	0.35	0.04	0.36
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	10	0.35	0.04	0.36
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	10	0.35	0.06	0.36
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	10	0.35	0.05	0.35
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	10	0.35	0.12	0.34
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE2	10	0.35	0.12	0.34
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG23	10	0.35	0.31	0.15
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG13	10	0.35	0.31	0.15
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG22	10	0.35	0.31	0.15
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG11	10	0.35	0.31	0.15
(2,736)	1:59:A:LEU:HD12	1:59:A:LEU:HG	10	0.35	0.02	0.35
(2,736)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.35	0.02	0.35
(2,736)	1:59:A:LEU:HD22	1:59:A:LEU:HG	10	0.35	0.02	0.35

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,736)	1:59:A:LEU:HD13	1:59:A:LEU:HG	10	0.35	0.02	0.35
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD11	10	0.35	0.07	0.32
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD12	10	0.35	0.07	0.32
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD13	10	0.35	0.07	0.32
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	10	0.34	0.08	0.32
(2,2160)	1:16:A:LEU:HD12	1:21:A:VAL:H	10	0.34	0.02	0.34
(2,2160)	1:16:A:LEU:HD13	1:21:A:VAL:H	10	0.34	0.02	0.34
(2,2160)	1:16:A:LEU:HD11	1:21:A:VAL:H	10	0.34	0.02	0.34
(2,3393)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	10	0.34	0.25	0.24
(2,3393)	1:37:A:VAL:HG11	2:109:B:LEU:HD11	10	0.34	0.25	0.24
(2,3393)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	10	0.34	0.25	0.24
(2,3393)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	10	0.34	0.25	0.24
(2,3393)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	10	0.34	0.25	0.24
(2,3393)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	10	0.34	0.25	0.24
(2,3393)	1:37:A:VAL:HG11	2:109:B:LEU:HD13	10	0.34	0.25	0.24
(2,3393)	1:37:A:VAL:HG12	2:109:B:LEU:HD13	10	0.34	0.25	0.24
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG13	10	0.34	0.37	0.23
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG11	10	0.34	0.37	0.23
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG12	10	0.34	0.37	0.23
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG22	10	0.34	0.37	0.23
(2,3509)	2:159:B:ILE:HG21	1:10:A:ILE:HG12	10	0.34	0.35	0.22
(2,3509)	2:159:B:ILE:HG22	1:10:A:ILE:HG12	10	0.34	0.35	0.22
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	10	0.34	0.07	0.34
(2,439)	1:16:A:LEU:HD23	1:13:A:ALA:HA	10	0.34	0.07	0.34
(2,439)	1:16:A:LEU:HD21	1:13:A:ALA:HA	10	0.34	0.07	0.34
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	10	0.34	0.03	0.35
(2,3396)	1:39:A:VAL:HG21	2:109:B:LEU:HD13	10	0.34	0.07	0.34
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	10	0.34	0.07	0.34
(2,3396)	1:39:A:VAL:HG21	2:109:B:LEU:HD12	10	0.34	0.07	0.34
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD22	10	0.34	0.07	0.34
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	10	0.34	0.07	0.34
(2,2714)	2:110:B:ALA:HB1	2:123:B:ILE:H	10	0.34	0.11	0.34
(2,2714)	2:110:B:ALA:HB3	2:123:B:ILE:H	10	0.34	0.11	0.34
(2,587)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	10	0.33	0.06	0.36
(2,587)	1:37:A:VAL:HG22	2:112:B:LEU:HD23	10	0.33	0.06	0.36
(2,587)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	10	0.33	0.06	0.36
(2,587)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	10	0.33	0.06	0.36
(2,587)	1:37:A:VAL:HG22	2:112:B:LEU:HD21	10	0.33	0.06	0.36
(2,587)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	10	0.33	0.06	0.36
(2,587)	1:37:A:VAL:HG23	2:112:B:LEU:HD21	10	0.33	0.06	0.36
(2,587)	1:37:A:VAL:HG21	2:112:B:LEU:HD21	10	0.33	0.06	0.36
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG22	10	0.33	0.05	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG23	10	0.33	0.05	0.34
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG21	10	0.33	0.05	0.34
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG13	10	0.33	0.37	0.22
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG11	10	0.33	0.37	0.22
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG12	10	0.33	0.37	0.22
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG22	10	0.33	0.37	0.22
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	10	0.33	0.07	0.36
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	10	0.33	0.04	0.33
(2,391)	1:10:A:ILE:HG22	2:159:B:ILE:HG12	10	0.33	0.13	0.36
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	10	0.33	0.13	0.36
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG23	10	0.33	0.05	0.34
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG21	10	0.33	0.05	0.34
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG22	10	0.33	0.05	0.34
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.32	0.01	0.33
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG12	10	0.32	0.01	0.33
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG13	10	0.32	0.01	0.33
(2,919)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	10	0.32	0.05	0.3
(2,919)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	10	0.32	0.05	0.3
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	10	0.32	0.03	0.32
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG21	10	0.32	0.03	0.33
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG23	10	0.32	0.03	0.33
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG22	10	0.32	0.03	0.33
(2,3388)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	10	0.32	0.25	0.22
(2,3388)	1:37:A:VAL:HG11	2:109:B:LEU:HD11	10	0.32	0.25	0.22
(2,3388)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	10	0.32	0.25	0.22
(2,3388)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	10	0.32	0.25	0.22
(2,3388)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	10	0.32	0.25	0.22
(2,3388)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	10	0.32	0.25	0.22
(2,3388)	1:37:A:VAL:HG11	2:109:B:LEU:HD13	10	0.32	0.25	0.22
(2,3388)	1:37:A:VAL:HG12	2:109:B:LEU:HD13	10	0.32	0.25	0.22
(2,3331)	1:14:A:LEU:HD23	2:159:B:ILE:HA	10	0.32	0.04	0.32
(2,3331)	1:14:A:LEU:HD22	2:159:B:ILE:HA	10	0.32	0.04	0.32
(2,3331)	1:14:A:LEU:HD21	2:159:B:ILE:HA	10	0.32	0.04	0.32
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB1	10	0.32	0.02	0.32
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB3	10	0.32	0.02	0.32
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB2	10	0.32	0.02	0.32
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.32	0.02	0.32
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	10	0.31	0.1	0.32
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB3	10	0.31	0.1	0.32
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	10	0.31	0.1	0.32
(2,1381)	1:23:A:VAL:HG11	1:48:A:ALA:HB1	10	0.31	0.1	0.32
(2,1381)	1:23:A:VAL:HG11	1:48:A:ALA:HB2	10	0.31	0.1	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1381)	1:23:A:VAL:HG13	1:48:A:ALA:HB2	10	0.31	0.1	0.32
(2,657)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	10	0.31	0.04	0.31
(2,657)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	10	0.31	0.04	0.31
(2,657)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	10	0.31	0.04	0.31
(2,3231)	2:159:B:ILE:HG23	2:159:B:ILE:H	10	0.31	0.04	0.32
(2,3231)	2:159:B:ILE:HG22	2:159:B:ILE:H	10	0.31	0.04	0.32
(2,3231)	2:159:B:ILE:HG21	2:159:B:ILE:H	10	0.31	0.04	0.32
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG11	10	0.31	0.05	0.31
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG12	10	0.31	0.05	0.31
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG13	10	0.31	0.05	0.31
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG11	10	0.31	0.02	0.3
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG12	10	0.31	0.02	0.3
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG13	10	0.31	0.02	0.3
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB2	10	0.31	0.1	0.29
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB1	10	0.31	0.1	0.29
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	10	0.31	0.03	0.32
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	10	0.31	0.02	0.31
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG13	10	0.31	0.02	0.31
(2,3507)	2:159:B:ILE:HG23	1:60:A:ILE:HG13	10	0.31	0.02	0.32
(2,3507)	2:159:B:ILE:HG22	1:60:A:ILE:HG13	10	0.31	0.02	0.32
(2,3507)	2:159:B:ILE:HG21	1:60:A:ILE:HG13	10	0.31	0.02	0.32
(2,3120)	2:147:B:ASN:HB3	2:148:B:GLY:H	10	0.31	0.07	0.31
(2,3120)	2:147:B:ASN:HB2	2:148:B:GLY:H	10	0.31	0.07	0.31
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.31	0.01	0.31
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.31	0.19	0.23
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.3	0.01	0.31
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	10	0.3	0.02	0.3
(2,1532)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	10	0.3	0.02	0.3
(2,2558)	1:59:A:LEU:HD12	1:59:A:LEU:HG	10	0.3	0.01	0.31
(2,2558)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.3	0.01	0.31
(2,2558)	1:59:A:LEU:HD22	1:59:A:LEU:HG	10	0.3	0.01	0.31
(2,2558)	1:59:A:LEU:HD13	1:59:A:LEU:HG	10	0.3	0.01	0.31
(2,3260)	2:163:B:ALA:HB3	2:163:B:ALA:HA	10	0.3	0.02	0.3
(2,3260)	2:163:B:ALA:HB1	2:163:B:ALA:HA	10	0.3	0.02	0.3
(2,3260)	2:163:B:ALA:HB2	2:163:B:ALA:HA	10	0.3	0.02	0.3
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB2	10	0.3	0.1	0.29
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB1	10	0.3	0.1	0.29
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB3	10	0.3	0.1	0.29
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	10	0.3	0.03	0.29
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB2	10	0.3	0.03	0.29
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	10	0.3	0.01	0.3
(2,2372)	1:37:A:VAL:HG21	2:112:B:LEU:HG	10	0.3	0.01	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2372)	1:37:A:VAL:HG22	2:112:B:LEU:HG	10	0.3	0.01	0.3
(2,2372)	1:37:A:VAL:HG23	2:112:B:LEU:HG	10	0.3	0.01	0.3
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	10	0.3	0.02	0.29
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	10	0.29	0.02	0.3
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB1	10	0.29	0.02	0.3
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB3	10	0.29	0.02	0.3
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	10	0.29	0.08	0.31
(2,620)	1:40:A:GLU:HG3	1:43:A:TRP:HD1	10	0.29	0.08	0.31
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	10	0.29	0.09	0.28
(2,2204)	1:20:A:GLU:HG2	1:19:A:ASP:H	10	0.29	0.12	0.31
(2,2204)	1:20:A:GLU:HG3	1:19:A:ASP:H	10	0.29	0.12	0.31
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	10	0.29	0.13	0.26
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	10	0.29	0.07	0.29
(2,2162)	1:16:A:LEU:HD23	1:13:A:ALA:HA	10	0.29	0.07	0.29
(2,2162)	1:16:A:LEU:HD21	1:13:A:ALA:HA	10	0.29	0.07	0.29
(2,1712)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	10	0.29	0.05	0.27
(2,1712)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	10	0.29	0.05	0.27
(2,3403)	1:59:A:LEU:HD11	2:159:B:ILE:HB	10	0.29	0.03	0.29
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	10	0.29	0.03	0.29
(2,3405)	1:59:A:LEU:HD11	2:159:B:ILE:HB	10	0.29	0.03	0.29
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	10	0.29	0.03	0.29
(2,3497)	1:59:A:LEU:HD11	2:159:B:ILE:HB	10	0.29	0.03	0.29
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	10	0.29	0.03	0.29
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD2	10	0.28	0.07	0.25
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD3	10	0.28	0.07	0.25
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	10	0.28	0.01	0.28
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	10	0.28	0.03	0.3
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG11	10	0.28	0.03	0.3
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG13	10	0.28	0.03	0.3
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	10	0.28	0.02	0.29
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD2	10	0.28	0.02	0.29
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.28	0.0	0.28
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG22	10	0.28	0.01	0.28
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG21	10	0.28	0.01	0.28
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG23	10	0.28	0.01	0.28
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.28	0.01	0.28
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	10	0.28	0.05	0.29
(2,3253)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.28	0.01	0.28
(2,3253)	2:162:B:LEU:HD22	2:162:B:LEU:HG	10	0.28	0.01	0.28
(2,3253)	2:162:B:LEU:HD12	2:162:B:LEU:HG	10	0.28	0.01	0.28
(2,3253)	2:162:B:LEU:HD23	2:162:B:LEU:HG	10	0.28	0.01	0.28
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	10	0.28	0.04	0.28

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,389)	1:10:A:ILE:HD12	1:7:A:LEU:HG	10	0.27	0.01	0.28
(2,389)	1:10:A:ILE:HD11	1:7:A:LEU:HG	10	0.27	0.01	0.28
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG22	10	0.27	0.02	0.26
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG21	10	0.27	0.02	0.26
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG23	10	0.27	0.02	0.26
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	10	0.27	0.05	0.26
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB3	10	0.27	0.05	0.26
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	10	0.27	0.04	0.29
(2,2969)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.27	0.04	0.29
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	10	0.27	0.02	0.27
(2,680)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	10	0.27	0.02	0.27
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG22	10	0.27	0.01	0.26
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG21	10	0.27	0.01	0.26
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG23	10	0.27	0.01	0.26
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	10	0.27	0.04	0.29
(2,2970)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.27	0.04	0.29
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	10	0.27	0.01	0.27
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD11	10	0.26	0.07	0.24
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD12	10	0.26	0.07	0.24
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD13	10	0.26	0.07	0.24
(2,1613)	2:101:B:MET:HE3	2:101:B:MET:HG2	10	0.26	0.08	0.26
(2,1613)	2:101:B:MET:HE2	2:101:B:MET:HG2	10	0.26	0.08	0.26
(2,1613)	2:101:B:MET:HE2	2:101:B:MET:HG3	10	0.26	0.08	0.26
(2,1081)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	10	0.26	0.07	0.26
(2,1081)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	10	0.26	0.07	0.26
(2,1081)	2:142:B:VAL:HG12	2:107:B:TYR:HE2	10	0.26	0.07	0.26
(2,3049)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	10	0.26	0.07	0.26
(2,3049)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	10	0.26	0.07	0.26
(2,3049)	2:142:B:VAL:HG12	2:107:B:TYR:HE2	10	0.26	0.07	0.26
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	10	0.26	0.04	0.26
(2,2209)	1:21:A:VAL:HG12	1:19:A:ASP:H	10	0.26	0.03	0.26
(2,2209)	1:21:A:VAL:HG13	1:19:A:ASP:H	10	0.26	0.03	0.26
(2,1228)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.26	0.01	0.26
(2,1228)	2:162:B:LEU:HD22	2:162:B:LEU:HG	10	0.26	0.01	0.26
(2,1228)	2:162:B:LEU:HD12	2:162:B:LEU:HG	10	0.26	0.01	0.26
(2,1228)	2:162:B:LEU:HD23	2:162:B:LEU:HG	10	0.26	0.01	0.26
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	10	0.26	0.03	0.25
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD2	10	0.26	0.03	0.25
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	10	0.26	0.02	0.26
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	10	0.26	0.04	0.28
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	10	0.26	0.01	0.26
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	10	0.26	0.04	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	10	0.25	0.02	0.25
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG11	10	0.25	0.02	0.25
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG12	10	0.25	0.02	0.25
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG13	10	0.25	0.02	0.25
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD13	10	0.25	0.05	0.25
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD11	10	0.25	0.05	0.25
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD12	10	0.25	0.05	0.25
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	10	0.25	0.05	0.27
(2,2238)	1:23:A:VAL:HG12	1:51:A:LEU:H	10	0.25	0.05	0.27
(2,2238)	1:23:A:VAL:HG11	1:51:A:LEU:H	10	0.25	0.05	0.27
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	10	0.25	0.04	0.26
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG23	10	0.25	0.04	0.26
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	10	0.25	0.02	0.24
(2,683)	1:50:A:ALA:HB2	1:54:A:VAL:HG22	10	0.25	0.08	0.24
(2,683)	1:50:A:ALA:HB3	1:54:A:VAL:HG23	10	0.25	0.08	0.24
(2,683)	1:50:A:ALA:HB1	1:54:A:VAL:HG21	10	0.25	0.08	0.24
(2,683)	1:50:A:ALA:HB1	1:54:A:VAL:HG12	10	0.25	0.08	0.24
(2,683)	1:50:A:ALA:HB1	1:54:A:VAL:HG22	10	0.25	0.08	0.24
(2,683)	1:50:A:ALA:HB3	1:54:A:VAL:HG22	10	0.25	0.08	0.24
(2,683)	1:50:A:ALA:HB2	1:54:A:VAL:HG23	10	0.25	0.08	0.24
(2,683)	1:50:A:ALA:HB3	1:54:A:VAL:HG11	10	0.25	0.08	0.24
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	10	0.25	0.04	0.26
(2,1023)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.25	0.04	0.26
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	10	0.25	0.01	0.25
(2,1234)	2:163:B:ALA:HB3	2:163:B:ALA:HA	10	0.25	0.03	0.24
(2,1234)	2:163:B:ALA:HB1	2:163:B:ALA:HA	10	0.25	0.03	0.24
(2,1234)	2:163:B:ALA:HB2	2:163:B:ALA:HA	10	0.25	0.03	0.24
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	10	0.25	0.01	0.25
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG22	10	0.25	0.01	0.24
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG21	10	0.25	0.01	0.24
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG23	10	0.25	0.01	0.24
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	10	0.25	0.01	0.25
(2,3504)	1:59:A:LEU:HD11	2:159:B:ILE:HG21	10	0.25	0.06	0.26
(2,3504)	1:59:A:LEU:HD11	2:159:B:ILE:HG22	10	0.25	0.06	0.26
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	10	0.25	0.06	0.26
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG23	10	0.25	0.06	0.26
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	10	0.25	0.06	0.26
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD11	10	0.24	0.1	0.18
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD13	10	0.24	0.1	0.18
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD12	10	0.24	0.1	0.18
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	10	0.24	0.05	0.23
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	10	0.24	0.03	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD12	10	0.24	0.03	0.24
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD11	10	0.24	0.03	0.24
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	10	0.24	0.04	0.23
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB3	10	0.24	0.03	0.24
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB2	10	0.24	0.03	0.24
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	10	0.24	0.01	0.24
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB2	10	0.24	0.02	0.23
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB3	10	0.24	0.02	0.23
(2,2552)	1:59:A:LEU:HD12	1:59:A:LEU:HG	10	0.23	0.01	0.24
(2,2552)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.23	0.01	0.24
(2,2552)	1:59:A:LEU:HD22	1:59:A:LEU:HG	10	0.23	0.01	0.24
(2,2552)	1:59:A:LEU:HD13	1:59:A:LEU:HG	10	0.23	0.01	0.24
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	10	0.23	0.02	0.24
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG22	10	0.23	0.01	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG12	10	0.23	0.01	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG21	10	0.23	0.01	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG23	10	0.23	0.01	0.23
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	10	0.23	0.02	0.24
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	10	0.23	0.04	0.24
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB2	10	0.23	0.04	0.24
(2,3018)	2:139:B:LEU:HD13	2:138:B:ARG:H	10	0.23	0.02	0.23
(2,3018)	2:139:B:LEU:HD11	2:138:B:ARG:H	10	0.23	0.02	0.23
(2,3018)	2:139:B:LEU:HD12	2:138:B:ARG:H	10	0.23	0.02	0.23
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	10	0.23	0.04	0.24
(2,756)	1:65:A:ALA:HB1	1:65:A:ALA:HA	10	0.23	0.04	0.24
(2,2098)	1:10:A:ILE:HD12	1:7:A:LEU:HG	10	0.23	0.01	0.23
(2,2098)	1:10:A:ILE:HD11	1:7:A:LEU:HG	10	0.23	0.01	0.23
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	10	0.23	0.03	0.22
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD11	10	0.23	0.06	0.23
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD13	10	0.23	0.06	0.23
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD12	10	0.23	0.06	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	10	0.23	0.0	0.23
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	10	0.23	0.03	0.22
(2,2543)	1:58:A:SER:HB2	1:59:A:LEU:HG	10	0.23	0.03	0.22
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	10	0.22	0.07	0.2
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.22	0.0	0.22
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	10	0.22	0.04	0.23
(2,1610)	1:65:A:ALA:HB1	1:65:A:ALA:HA	10	0.22	0.04	0.23
(2,1944)	2:154:B:VAL:HG12	2:154:B:VAL:HA	10	0.22	0.17	0.15
(2,1944)	2:154:B:VAL:HG22	2:154:B:VAL:HA	10	0.22	0.17	0.15
(2,1944)	2:154:B:VAL:HG13	2:154:B:VAL:HA	10	0.22	0.17	0.15
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	10	0.22	0.04	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,738)	1:59:A:LEU:HD12	1:59:A:LEU:HG	10	0.22	0.02	0.22
(2,738)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.22	0.02	0.22
(2,738)	1:59:A:LEU:HD22	1:59:A:LEU:HG	10	0.22	0.02	0.22
(2,738)	1:59:A:LEU:HD13	1:59:A:LEU:HG	10	0.22	0.02	0.22
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	10	0.22	0.03	0.21
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	10	0.22	0.01	0.22
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	10	0.22	0.02	0.22
(2,658)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	10	0.22	0.03	0.21
(2,658)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	10	0.22	0.03	0.21
(2,658)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	10	0.22	0.03	0.21
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD22	10	0.21	0.03	0.22
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	10	0.21	0.03	0.22
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD23	10	0.21	0.03	0.22
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.21	0.01	0.21
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	10	0.21	0.02	0.22
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG22	10	0.21	0.02	0.22
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.21	0.01	0.21
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB3	10	0.21	0.05	0.2
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB2	10	0.21	0.05	0.2
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG21	10	0.21	0.02	0.2
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG23	10	0.21	0.02	0.2
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG22	10	0.21	0.02	0.2
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE2	10	0.21	0.08	0.19
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE1	10	0.21	0.08	0.19
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	10	0.21	0.03	0.22
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	10	0.21	0.05	0.22
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	10	0.21	0.03	0.21
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	10	0.21	0.02	0.2
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD22	10	0.21	0.01	0.21
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD23	10	0.21	0.01	0.21
(2,1130)	2:146:B:LEU:HD22	2:146:B:LEU:HG	10	0.2	0.02	0.2
(2,1130)	2:146:B:LEU:HD11	2:146:B:LEU:HG	10	0.2	0.02	0.2
(2,1130)	2:146:B:LEU:HD13	2:146:B:LEU:HG	10	0.2	0.02	0.2
(2,1130)	2:146:B:LEU:HD12	2:146:B:LEU:HG	10	0.2	0.02	0.2
(2,2589)	1:62:A:ASN:HB2	1:43:A:TRP:HZ2	10	0.2	0.04	0.2
(2,2589)	1:62:A:ASN:HB3	1:43:A:TRP:HZ2	10	0.2	0.04	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG22	10	0.2	0.01	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG23	10	0.2	0.01	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG21	10	0.2	0.01	0.2
(2,2073)	1:7:A:LEU:HD11	1:7:A:LEU:H	10	0.2	0.04	0.2
(2,2073)	1:7:A:LEU:HD12	1:7:A:LEU:H	10	0.2	0.04	0.2
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	10	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	10	0.2	0.03	0.2
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	10	0.2	0.03	0.19
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD22	10	0.2	0.03	0.2
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	10	0.2	0.03	0.2
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD23	10	0.2	0.03	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG22	10	0.2	0.01	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG23	10	0.2	0.01	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG21	10	0.2	0.01	0.2
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.2	0.01	0.2
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB1	10	0.2	0.05	0.21
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB3	10	0.2	0.05	0.21
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	10	0.2	0.05	0.18
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	10	0.2	0.05	0.18
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG21	10	0.2	0.05	0.18
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG11	10	0.2	0.01	0.2
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG13	10	0.2	0.01	0.2
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG22	10	0.2	0.01	0.2
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG12	10	0.2	0.01	0.2
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD11	10	0.19	0.06	0.2
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD13	10	0.19	0.06	0.2
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD12	10	0.19	0.06	0.2
(2,1179)	2:155:B:ILE:HG23	2:155:B:ILE:HB	10	0.19	0.02	0.2
(2,1179)	2:155:B:ILE:HG21	2:155:B:ILE:HB	10	0.19	0.02	0.2
(2,1179)	2:155:B:ILE:HG22	2:155:B:ILE:HB	10	0.19	0.02	0.2
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG12	10	0.19	0.02	0.19
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG13	10	0.19	0.02	0.19
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	10	0.19	0.02	0.19
(2,1536)	1:51:A:LEU:HD12	1:51:A:LEU:HG	10	0.19	0.03	0.2
(2,1536)	1:51:A:LEU:HD11	1:51:A:LEU:HG	10	0.19	0.03	0.2
(2,1536)	1:51:A:LEU:HD21	1:51:A:LEU:HG	10	0.19	0.03	0.2
(2,1536)	1:51:A:LEU:HD13	1:51:A:LEU:HG	10	0.19	0.03	0.2
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	10	0.19	0.0	0.19
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG22	10	0.19	0.02	0.18
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG21	10	0.19	0.02	0.18
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG23	10	0.19	0.02	0.18
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	10	0.19	0.01	0.19
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	10	0.19	0.06	0.16
(2,1230)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.19	0.01	0.18
(2,1230)	2:162:B:LEU:HD22	2:162:B:LEU:HG	10	0.19	0.01	0.18
(2,1230)	2:162:B:LEU:HD12	2:162:B:LEU:HG	10	0.19	0.01	0.18
(2,1230)	2:162:B:LEU:HD23	2:162:B:LEU:HG	10	0.19	0.01	0.18
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	10	0.18	0.01	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	10	0.18	0.04	0.19
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	10	0.18	0.03	0.18
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD2	10	0.18	0.03	0.18
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	10	0.18	0.04	0.17
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.18	0.01	0.18
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	10	0.18	0.04	0.18
(2,2862)	2:124:B:LYS:HE3	2:124:B:LYS:HD2	10	0.18	0.04	0.18
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	10	0.18	0.01	0.18
(2,1718)	2:121:B:LYS:HB2	2:121:B:LYS:HG2	10	0.18	0.01	0.18
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	10	0.18	0.03	0.18
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	10	0.18	0.04	0.18
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG13	10	0.18	0.02	0.18
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG12	10	0.18	0.02	0.18
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	10	0.18	0.03	0.16
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB2	10	0.18	0.03	0.16
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.18	0.0	0.18
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	10	0.18	0.02	0.17
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG22	10	0.17	0.01	0.18
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG23	10	0.17	0.01	0.18
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG21	10	0.17	0.01	0.18
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD13	10	0.17	0.03	0.18
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD12	10	0.17	0.03	0.18
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD11	10	0.17	0.03	0.18
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	10	0.17	0.01	0.17
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	10	0.17	0.07	0.14
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	10	0.17	0.02	0.16
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	10	0.17	0.08	0.13
(2,347)	1:2:A:ALA:HB1	1:7:A:LEU:HB2	10	0.17	0.08	0.13
(2,347)	1:2:A:ALA:HB2	1:7:A:LEU:HB2	10	0.17	0.08	0.13
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	10	0.17	0.03	0.17
(2,726)	1:58:A:SER:HB3	1:58:A:SER:HA	10	0.17	0.03	0.17
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	10	0.17	0.04	0.17
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.17	0.01	0.17
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	10	0.16	0.09	0.12
(2,344)	1:2:A:ALA:HB1	1:7:A:LEU:HB2	10	0.16	0.09	0.12
(2,344)	1:2:A:ALA:HB2	1:7:A:LEU:HB2	10	0.16	0.09	0.12
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	10	0.16	0.02	0.17
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB2	10	0.16	0.02	0.17
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	10	0.16	0.01	0.16
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	10	0.16	0.02	0.16
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB1	10	0.16	0.02	0.16
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB3	10	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.16	0.01	0.16
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG12	10	0.16	0.01	0.16
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG13	10	0.16	0.01	0.16
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	10	0.16	0.02	0.16
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	10	0.16	0.03	0.15
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB2	10	0.16	0.03	0.15
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD23	10	0.16	0.03	0.16
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD21	10	0.16	0.03	0.16
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD12	10	0.16	0.03	0.16
(2,3248)	2:162:B:LEU:HB3	2:162:B:LEU:HD21	10	0.16	0.03	0.16
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD13	10	0.16	0.03	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	10	0.16	0.0	0.16
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	10	0.16	0.02	0.16
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB2	10	0.15	0.02	0.15
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB3	10	0.15	0.02	0.15
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	10	0.15	0.03	0.14
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	10	0.15	0.03	0.16
(2,1568)	1:58:A:SER:HB3	1:58:A:SER:HA	10	0.15	0.03	0.16
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	10	0.15	0.01	0.16
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	10	0.15	0.02	0.15
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	10	0.15	0.02	0.15
(2,2477)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	10	0.15	0.02	0.15
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	10	0.15	0.02	0.15
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	10	0.15	0.02	0.15
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	10	0.15	0.02	0.15
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	10	0.15	0.01	0.15
(2,588)	1:37:A:VAL:HG21	2:112:B:LEU:HG	10	0.15	0.01	0.15
(2,588)	1:37:A:VAL:HG22	2:112:B:LEU:HG	10	0.15	0.01	0.15
(2,588)	1:37:A:VAL:HG23	2:112:B:LEU:HG	10	0.15	0.01	0.15
(2,3250)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.15	0.01	0.15
(2,3250)	2:162:B:LEU:HD22	2:162:B:LEU:HG	10	0.15	0.01	0.15
(2,3250)	2:162:B:LEU:HD12	2:162:B:LEU:HG	10	0.15	0.01	0.15
(2,3250)	2:162:B:LEU:HD23	2:162:B:LEU:HG	10	0.15	0.01	0.15
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG11	10	0.15	0.01	0.15
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG13	10	0.15	0.01	0.15
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG22	10	0.15	0.01	0.15
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG12	10	0.15	0.01	0.15
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	10	0.15	0.02	0.15
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	10	0.14	0.02	0.15
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB1	10	0.14	0.02	0.15
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB3	10	0.14	0.02	0.15
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG22	10	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG21	10	0.14	0.02	0.14
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG23	10	0.14	0.02	0.14
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	10	0.14	0.01	0.14
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	10	0.14	0.01	0.14
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	10	0.14	0.03	0.14
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	10	0.14	0.01	0.14
(2,2568)	1:60:A:ILE:HG12	1:60:A:ILE:HD13	10	0.14	0.01	0.14
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	10	0.14	0.01	0.14
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG12	10	0.14	0.01	0.14
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG13	10	0.14	0.01	0.14
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	10	0.13	0.01	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG13	10	0.13	0.01	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG21	10	0.13	0.01	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG12	10	0.13	0.01	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG11	10	0.13	0.01	0.13
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	10	0.13	0.02	0.12
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	10	0.12	0.01	0.12
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	10	0.12	0.01	0.12
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	10	0.11	0.01	0.11
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	9	1.27	0.11	1.26
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD23	9	1.2	0.26	1.25
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD21	9	1.2	0.26	1.25
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	9	1.19	0.49	1.33
(2,795)	2:104:B:VAL:HG12	2:103:B:TYR:HA	9	1.19	0.49	1.33
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD23	9	1.18	0.26	1.23
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD21	9	1.18	0.26	1.23
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	9	1.11	0.51	1.36
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	9	1.11	0.51	1.36
(2,752)	1:61:A:CYS:HB2	1:60:A:ILE:HG21	9	1.11	0.51	1.36
(2,3300)	1:2:A:ALA:HB3	2:152:B:GLU:HG3	9	1.08	0.5	1.01
(2,3300)	1:2:A:ALA:HB1	2:152:B:GLU:HG3	9	1.08	0.5	1.01
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	9	1.06	0.11	1.05
(2,1266)	1:1:A:MET:HG3	2:152:B:GLU:HG3	9	1.02	0.49	1.03
(2,1266)	1:1:A:MET:HG2	2:152:B:GLU:HG3	9	1.02	0.49	1.03
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	9	0.95	0.17	0.93
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	9	0.89	0.17	0.85
(2,1132)	2:143:B:ILE:HA	2:146:B:LEU:HD12	9	0.89	0.17	0.85
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	9	0.86	0.17	0.84
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD23	9	0.86	0.26	0.9
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD21	9	0.86	0.26	0.9
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	9	0.72	0.23	0.85
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG12	9	0.68	0.5	0.46

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1996)	2:162:B:LEU:HA	2:165:B:VAL:HG22	9	0.68	0.5	0.46
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG11	9	0.68	0.5	0.46
(2,555)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	9	0.65	0.12	0.61
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	9	0.65	0.12	0.61
(2,555)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	9	0.65	0.12	0.61
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE3	9	0.65	0.12	0.61
(2,1898)	2:146:B:LEU:HD13	2:151:B:ILE:HG13	9	0.63	0.16	0.66
(2,1898)	2:146:B:LEU:HD12	2:151:B:ILE:HG13	9	0.63	0.16	0.66
(2,1898)	2:146:B:LEU:HD11	2:151:B:ILE:HG13	9	0.63	0.16	0.66
(2,2976)	2:134:B:ALA:HB3	2:135:B:ASP:HB2	9	0.61	0.45	0.35
(2,2976)	2:134:B:ALA:HB2	2:135:B:ASP:HB3	9	0.61	0.45	0.35
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG12	9	0.6	0.11	0.61
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG13	9	0.6	0.11	0.61
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG11	9	0.6	0.11	0.61
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	9	0.6	0.1	0.58
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	9	0.58	0.16	0.63
(2,2282)	1:27:A:LYS:HG2	1:27:A:LYS:H	9	0.58	0.16	0.63
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG2	9	0.57	0.38	0.36
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG3	9	0.57	0.38	0.36
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	9	0.53	0.13	0.46
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD2	9	0.53	0.13	0.46
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	9	0.53	0.13	0.46
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD2	9	0.53	0.13	0.46
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD11	9	0.52	0.12	0.57
(2,3495)	2:156:B:ALA:HB1	1:7:A:LEU:HD13	9	0.52	0.12	0.57
(2,3495)	2:156:B:ALA:HB3	1:7:A:LEU:HD13	9	0.52	0.12	0.57
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD21	9	0.52	0.12	0.57
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	9	0.5	0.24	0.43
(2,827)	2:108:B:LEU:HD22	2:104:B:VAL:HB	9	0.5	0.24	0.43
(2,3025)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	9	0.48	0.08	0.45
(2,3025)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	9	0.48	0.08	0.45
(2,3025)	2:139:B:LEU:HD22	2:124:B:LYS:HE3	9	0.48	0.08	0.45
(2,2950)	2:132:B:ILE:HD13	2:130:B:VAL:H	9	0.46	0.1	0.51
(2,2950)	2:132:B:ILE:HD11	2:130:B:VAL:H	9	0.46	0.1	0.51
(2,1054)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	9	0.45	0.08	0.42
(2,1054)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	9	0.45	0.08	0.42
(2,1054)	2:139:B:LEU:HD22	2:124:B:LYS:HE3	9	0.45	0.08	0.42
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	9	0.44	0.03	0.44
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE2	9	0.44	0.03	0.44
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	9	0.44	0.03	0.44
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE2	9	0.44	0.03	0.44
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG21	9	0.4	0.07	0.37

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG23	9	0.4	0.07	0.37
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG22	9	0.4	0.07	0.37
(2,2945)	2:132:B:ILE:HD12	2:133:B:GLU:H	9	0.37	0.23	0.3
(2,2945)	2:132:B:ILE:HD13	2:133:B:GLU:H	9	0.37	0.23	0.3
(2,682)	1:50:A:ALA:HB1	1:46:A:LEU:HB3	9	0.34	0.23	0.26
(2,682)	1:50:A:ALA:HB2	1:46:A:LEU:HB2	9	0.34	0.23	0.26
(2,682)	1:50:A:ALA:HB3	1:46:A:LEU:HB3	9	0.34	0.23	0.26
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	9	0.32	0.1	0.28
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG11	9	0.31	0.04	0.33
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG12	9	0.31	0.04	0.33
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG13	9	0.31	0.04	0.33
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	9	0.29	0.24	0.22
(2,826)	2:108:B:LEU:HD22	2:104:B:VAL:HB	9	0.29	0.24	0.22
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	9	0.29	0.04	0.29
(2,1082)	2:142:B:VAL:HG13	2:103:B:TYR:HD2	9	0.29	0.03	0.3
(2,1082)	2:142:B:VAL:HG12	2:103:B:TYR:HD2	9	0.29	0.03	0.3
(2,1082)	2:142:B:VAL:HG11	2:103:B:TYR:HD2	9	0.29	0.03	0.3
(2,3261)	2:163:B:ALA:HB2	2:163:B:ALA:H	9	0.28	0.03	0.28
(2,3261)	2:163:B:ALA:HB3	2:163:B:ALA:H	9	0.28	0.03	0.28
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	9	0.28	0.06	0.3
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	9	0.28	0.08	0.28
(2,1742)	2:134:B:ALA:HB1	2:124:B:LYS:HA	9	0.27	0.09	0.23
(2,1742)	2:134:B:ALA:HB3	2:124:B:LYS:HA	9	0.27	0.09	0.23
(2,2388)	1:37:A:VAL:HG23	1:38:A:ASN:HB3	9	0.25	0.1	0.25
(2,2388)	1:37:A:VAL:HG22	1:38:A:ASN:HB3	9	0.25	0.1	0.25
(2,2388)	1:37:A:VAL:HG21	1:38:A:ASN:HB3	9	0.25	0.1	0.25
(2,2388)	1:38:A:ASN:HB2	1:39:A:VAL:HG22	9	0.25	0.1	0.25
(2,3364)	1:31:A:LEU:HD11	2:130:B:VAL:HA	9	0.25	0.13	0.19
(2,3364)	1:31:A:LEU:HD13	2:130:B:VAL:HA	9	0.25	0.13	0.19
(2,3364)	1:31:A:LEU:HD12	2:130:B:VAL:HA	9	0.25	0.13	0.19
(2,3364)	1:31:A:LEU:HD21	2:130:B:VAL:HA	9	0.25	0.13	0.19
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	9	0.25	0.03	0.26
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	9	0.24	0.07	0.25
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	9	0.23	0.08	0.21
(2,740)	1:59:A:LEU:HD12	1:56:A:ILE:HA	9	0.23	0.08	0.23
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	9	0.23	0.08	0.23
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG12	9	0.22	0.05	0.21
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG11	9	0.22	0.05	0.21
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG13	9	0.22	0.05	0.21
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	9	0.21	0.04	0.2
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	9	0.21	0.05	0.2
(2,213)	2:116:B:SER:H	2:117:B:SER:HB2	9	0.21	0.05	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	9	0.21	0.07	0.19
(2,1450)	1:33:A:LYS:HG2	1:33:A:LYS:HD3	9	0.2	0.02	0.21
(2,1450)	1:33:A:LYS:HG3	1:33:A:LYS:HD2	9	0.2	0.02	0.21
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	9	0.2	0.04	0.22
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG23	9	0.2	0.02	0.2
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG22	9	0.2	0.02	0.2
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	9	0.19	0.04	0.21
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	9	0.19	0.06	0.2
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	9	0.18	0.05	0.18
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	9	0.18	0.04	0.19
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB2	9	0.18	0.04	0.19
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG2	9	0.18	0.03	0.17
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG3	9	0.18	0.03	0.17
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	9	0.18	0.05	0.17
(2,3317)	1:8:A:ALA:HB1	2:109:B:LEU:HG	9	0.18	0.03	0.18
(2,3317)	1:8:A:ALA:HB2	2:109:B:LEU:HG	9	0.18	0.03	0.18
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD12	9	0.17	0.04	0.18
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD13	9	0.17	0.04	0.18
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD12	9	0.17	0.04	0.18
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD13	9	0.17	0.04	0.18
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG2	9	0.17	0.03	0.16
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG3	9	0.17	0.03	0.16
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	9	0.16	0.04	0.18
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	9	0.16	0.02	0.16
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG21	9	0.16	0.02	0.16
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG22	9	0.16	0.02	0.16
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG23	9	0.16	0.02	0.16
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	9	0.16	0.03	0.16
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB3	9	0.16	0.06	0.13
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB2	9	0.16	0.06	0.13
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB2	9	0.16	0.03	0.17
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB3	9	0.16	0.03	0.17
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB1	9	0.16	0.03	0.17
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	9	0.16	0.06	0.13
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	9	0.16	0.04	0.16
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	9	0.16	0.04	0.15
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	9	0.15	0.04	0.15
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	9	0.15	0.02	0.14
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	9	0.14	0.02	0.14
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	9	0.14	0.03	0.14
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD13	9	0.14	0.02	0.14
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD12	9	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD11	9	0.14	0.02	0.14
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	9	0.14	0.01	0.14
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB3	9	0.14	0.02	0.14
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB2	9	0.14	0.02	0.14
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB1	9	0.14	0.02	0.14
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	9	0.13	0.02	0.13
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	9	0.13	0.01	0.13
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB2	9	0.13	0.01	0.13
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB3	9	0.13	0.01	0.12
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB2	9	0.13	0.01	0.12
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB1	9	0.13	0.01	0.12
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG12	9	0.13	0.01	0.13
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG13	9	0.13	0.01	0.13
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG11	9	0.13	0.01	0.13
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	9	0.12	0.01	0.12
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	9	0.12	0.01	0.12
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	9	0.11	0.01	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG22	9	0.11	0.0	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG12	9	0.11	0.0	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG21	9	0.11	0.0	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG23	9	0.11	0.0	0.11
(2,2626)	2:101:B:MET:HE1	2:102:B:ARG:H	8	1.0	0.49	1.19
(2,2626)	2:101:B:MET:HE2	2:102:B:ARG:H	8	1.0	0.49	1.19
(2,2626)	2:101:B:MET:HE2	2:103:B:TYR:H	8	1.0	0.49	1.19
(2,2626)	2:101:B:MET:HE3	2:104:B:VAL:H	8	1.0	0.49	1.19
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.91	0.05	0.92
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.84	0.05	0.85
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	8	0.82	0.4	1.06
(2,3099)	2:146:B:LEU:HD12	2:149:B:LYS:HE3	8	0.78	0.25	0.77
(2,3099)	2:146:B:LEU:HD23	2:149:B:LYS:HE3	8	0.78	0.25	0.77
(2,1393)	1:24:A:THR:HG21	1:26:A:ASP:HB3	8	0.76	0.16	0.78
(2,1393)	1:24:A:THR:HG23	1:26:A:ASP:HB3	8	0.76	0.16	0.78
(2,1393)	1:24:A:THR:HG22	1:26:A:ASP:HB2	8	0.76	0.16	0.78
(2,1393)	1:24:A:THR:HG22	1:26:A:ASP:HB3	8	0.76	0.16	0.78
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.64	0.05	0.65
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB2	8	0.63	0.08	0.68
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB3	8	0.63	0.08	0.68
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	8	0.63	0.1	0.67
(2,569)	1:34:A:ALA:HB3	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,569)	1:34:A:ALA:HB2	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	8	0.63	0.1	0.67

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2341)	1:34:A:ALA:HB3	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,2341)	1:34:A:ALA:HB2	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	8	0.63	0.1	0.67
(2,3373)	1:34:A:ALA:HB3	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,3373)	1:34:A:ALA:HB2	2:125:B:LYS:HE2	8	0.63	0.1	0.67
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	8	0.62	0.32	0.48
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	8	0.62	0.32	0.48
(2,2318)	1:32:A:ILE:HD13	1:9:A:CYS:H	8	0.59	0.53	0.22
(2,2318)	1:32:A:ILE:HD12	1:9:A:CYS:H	8	0.59	0.53	0.22
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG21	8	0.59	0.6	0.14
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG22	8	0.59	0.6	0.14
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	8	0.53	0.33	0.34
(2,3296)	1:1:A:MET:HE1	2:156:B:ALA:HA	8	0.47	0.11	0.45
(2,3296)	1:1:A:MET:HE2	2:156:B:ALA:HA	8	0.47	0.11	0.45
(2,3296)	1:1:A:MET:HE3	2:156:B:ALA:HA	8	0.47	0.11	0.45
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	8	0.41	0.06	0.43
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.41	0.06	0.43
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD2	8	0.4	0.14	0.4
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD3	8	0.4	0.14	0.4
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	8	0.4	0.06	0.42
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.4	0.06	0.42
(2,2147)	1:15:A:ILE:HD13	2:103:B:TYR:HA	8	0.38	0.08	0.41
(2,2147)	1:15:A:ILE:HD11	2:103:B:TYR:HA	8	0.38	0.08	0.41
(2,2147)	1:15:A:ILE:HD12	2:103:B:TYR:HA	8	0.38	0.08	0.41
(2,3387)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	8	0.37	0.39	0.16
(2,3387)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	8	0.37	0.39	0.16
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB2	8	0.36	0.08	0.4
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB3	8	0.36	0.08	0.4
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	8	0.36	0.06	0.37
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.36	0.06	0.37
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD11	8	0.34	0.06	0.35
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD12	8	0.34	0.06	0.35
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD13	8	0.34	0.06	0.35
(2,357)	1:4:A:VAL:HG23	2:112:B:LEU:HA	8	0.34	0.13	0.32
(2,357)	1:4:A:VAL:HG22	2:112:B:LEU:HA	8	0.34	0.13	0.32
(2,357)	1:4:A:VAL:HG11	2:112:B:LEU:HA	8	0.34	0.13	0.32
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	8	0.33	0.02	0.32
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	8	0.31	0.12	0.34
(2,3301)	1:2:A:ALA:HB3	2:152:B:GLU:HA	8	0.3	0.08	0.32
(2,3301)	1:2:A:ALA:HB1	2:152:B:GLU:HA	8	0.3	0.08	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2258)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	8	0.29	0.15	0.22
(2,2258)	1:25:A:GLU:HG2	1:48:A:ALA:HB3	8	0.29	0.15	0.22
(2,2258)	1:25:A:GLU:HG3	1:48:A:ALA:HB1	8	0.29	0.15	0.22
(2,2258)	1:25:A:GLU:HG3	1:48:A:ALA:HB3	8	0.29	0.15	0.22
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	8	0.28	0.09	0.29
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG12	8	0.28	0.09	0.29
(2,3307)	1:4:A:VAL:HG23	2:112:B:LEU:HA	8	0.27	0.1	0.24
(2,3307)	1:4:A:VAL:HG22	2:112:B:LEU:HA	8	0.27	0.1	0.24
(2,3307)	1:4:A:VAL:HG11	2:112:B:LEU:HA	8	0.27	0.1	0.24
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	8	0.27	0.1	0.27
(2,2851)	2:123:B:ILE:HG22	2:126:B:ILE:H	8	0.27	0.11	0.3
(2,2851)	2:123:B:ILE:HG21	2:126:B:ILE:H	8	0.27	0.11	0.3
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB2	8	0.26	0.08	0.3
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB3	8	0.26	0.08	0.3
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	8	0.25	0.25	0.16
(2,2683)	2:108:B:LEU:HD22	2:104:B:VAL:HB	8	0.25	0.25	0.16
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.25	0.05	0.25
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	8	0.25	0.05	0.26
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	8	0.24	0.11	0.19
(2,2329)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	8	0.24	0.11	0.19
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE3	8	0.24	0.11	0.19
(2,2329)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	8	0.24	0.11	0.19
(2,2842)	2:123:B:ILE:HG23	2:139:B:LEU:H	8	0.23	0.1	0.22
(2,2842)	2:123:B:ILE:HG21	2:139:B:LEU:H	8	0.23	0.1	0.22
(2,2842)	2:123:B:ILE:HG22	2:139:B:LEU:H	8	0.23	0.1	0.22
(2,2557)	1:59:A:LEU:HD12	1:56:A:ILE:HA	8	0.21	0.08	0.2
(2,2557)	1:59:A:LEU:HD13	1:56:A:ILE:HA	8	0.21	0.08	0.2
(2,2561)	1:59:A:LEU:HD12	1:56:A:ILE:HA	8	0.21	0.08	0.2
(2,2561)	1:59:A:LEU:HD13	1:56:A:ILE:HA	8	0.21	0.08	0.2
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	8	0.2	0.09	0.18
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG22	8	0.2	0.09	0.18
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	8	0.2	0.03	0.2
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	8	0.19	0.07	0.16
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE2	8	0.19	0.07	0.16
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE2	8	0.18	0.08	0.16
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE1	8	0.18	0.08	0.16
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	8	0.18	0.03	0.18
(2,2324)	1:32:A:ILE:HD12	1:31:A:LEU:H	8	0.18	0.07	0.17
(2,2324)	1:32:A:ILE:HD13	1:31:A:LEU:H	8	0.18	0.07	0.17
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	8	0.18	0.05	0.2
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG13	8	0.18	0.05	0.16
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG11	8	0.18	0.05	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG12	8	0.18	0.05	0.16
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	8	0.17	0.03	0.18
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	8	0.17	0.03	0.17
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG2	8	0.16	0.04	0.16
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG3	8	0.16	0.04	0.16
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	8	0.16	0.04	0.16
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB3	8	0.16	0.03	0.15
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB2	8	0.16	0.03	0.15
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG2	8	0.15	0.02	0.15
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG3	8	0.15	0.02	0.15
(2,2244)	1:24:A:THR:HG23	1:24:A:THR:HA	8	0.15	0.02	0.15
(2,2244)	1:24:A:THR:HG22	1:24:A:THR:HA	8	0.15	0.02	0.15
(2,2244)	1:24:A:THR:HG21	1:24:A:THR:HA	8	0.15	0.02	0.15
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG23	8	0.14	0.02	0.14
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG21	8	0.14	0.02	0.14
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG22	8	0.14	0.02	0.14
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	8	0.13	0.03	0.12
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	8	0.13	0.01	0.13
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG23	8	0.13	0.03	0.12
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG22	8	0.13	0.03	0.12
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG21	8	0.13	0.03	0.12
(2,793)	2:104:B:VAL:HG11	2:104:B:VAL:HB	8	0.12	0.01	0.12
(2,793)	2:104:B:VAL:HG12	2:104:B:VAL:HB	8	0.12	0.01	0.12
(2,793)	2:104:B:VAL:HG23	2:104:B:VAL:HB	8	0.12	0.01	0.12
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG21	8	0.12	0.01	0.12
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG13	8	0.12	0.01	0.12
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG12	8	0.12	0.01	0.12
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	8	0.11	0.01	0.11
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG22	8	0.11	0.01	0.11
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG21	8	0.11	0.01	0.11
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG23	8	0.11	0.01	0.11
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	7	1.24	0.12	1.24
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	7	1.24	0.12	1.24
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	7	0.93	0.13	0.96
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	7	0.93	0.13	0.96
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	7	0.93	0.13	0.96
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	7	0.93	0.13	0.96
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	7	0.93	0.13	0.96
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	7	0.93	0.13	0.96
(2,1843)	2:139:B:LEU:HD13	2:143:B:ILE:HD12	7	0.91	0.29	1.03
(2,1843)	2:139:B:LEU:HD12	2:143:B:ILE:HD13	7	0.91	0.29	1.03
(2,1843)	2:139:B:LEU:HD13	2:143:B:ILE:HD11	7	0.91	0.29	1.03

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1843)	2:139:B:LEU:HD12	2:143:B:ILE:HD11	7	0.91	0.29	1.03
(2,1843)	2:139:B:LEU:HD11	2:143:B:ILE:HD13	7	0.91	0.29	1.03
(2,1994)	2:161:B:LYS:HE3	2:161:B:LYS:HB2	7	0.69	0.37	0.55
(2,1994)	2:161:B:LYS:HE2	2:161:B:LYS:HB3	7	0.69	0.37	0.55
(2,314)	2:153:B:ASP:H	2:154:B:VAL:HG21	7	0.67	0.27	0.77
(2,314)	2:153:B:ASP:H	2:151:B:ILE:HG22	7	0.67	0.27	0.77
(2,3488)	2:152:B:GLU:HB2	1:4:A:VAL:HG23	7	0.61	0.33	0.51
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	7	0.61	0.33	0.51
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG23	7	0.61	0.33	0.51
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG21	7	0.52	0.22	0.61
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG22	7	0.52	0.22	0.61
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	7	0.47	0.06	0.46
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	7	0.47	0.06	0.46
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.47	0.06	0.46
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	7	0.47	0.06	0.46
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	7	0.47	0.06	0.46
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.47	0.06	0.46
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	7	0.47	0.06	0.46
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	7	0.47	0.06	0.46
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.47	0.06	0.46
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	7	0.47	0.06	0.46
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	7	0.47	0.06	0.46
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.47	0.06	0.46
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	7	0.47	0.06	0.46
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	7	0.47	0.06	0.46
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.47	0.06	0.46
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	7	0.45	0.01	0.45
(2,558)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	7	0.43	0.12	0.44
(2,558)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	7	0.43	0.12	0.44
(2,1873)	2:143:B:ILE:HD11	2:142:B:VAL:HG11	7	0.42	0.25	0.59
(2,1873)	2:143:B:ILE:HD12	2:142:B:VAL:HG11	7	0.42	0.25	0.59
(2,1873)	2:143:B:ILE:HD12	2:142:B:VAL:HG12	7	0.42	0.25	0.59
(2,1873)	2:143:B:ILE:HD12	2:142:B:VAL:HG13	7	0.42	0.25	0.59
(2,1873)	2:143:B:ILE:HD11	2:142:B:VAL:HG12	7	0.42	0.25	0.59
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	7	0.38	0.16	0.43
(2,567)	1:34:A:ALA:HB1	2:126:B:ILE:HD12	7	0.37	0.19	0.35
(2,567)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	7	0.37	0.19	0.35
(2,567)	1:34:A:ALA:HB3	2:126:B:ILE:HG22	7	0.37	0.19	0.35
(2,567)	1:34:A:ALA:HB2	2:126:B:ILE:HG22	7	0.37	0.19	0.35
(2,2346)	1:34:A:ALA:HB1	2:126:B:ILE:HD12	7	0.37	0.19	0.35
(2,2346)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	7	0.37	0.19	0.35
(2,2346)	1:34:A:ALA:HB3	2:126:B:ILE:HG22	7	0.37	0.19	0.35

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2346)	1:34:A:ALA:HB2	2:126:B:ILE:HG22	7	0.37	0.19	0.35
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG13	7	0.34	0.42	0.15
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG11	7	0.34	0.42	0.15
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG12	7	0.34	0.42	0.15
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG22	7	0.34	0.42	0.15
(2,2328)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	7	0.33	0.12	0.34
(2,2328)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	7	0.33	0.12	0.34
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	7	0.29	0.01	0.29
(2,1105)	2:143:B:ILE:HG23	2:143:B:ILE:HD13	7	0.29	0.39	0.14
(2,1105)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	7	0.29	0.39	0.14
(2,1105)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	7	0.29	0.39	0.14
(2,3074)	2:143:B:ILE:HG23	2:143:B:ILE:HD13	7	0.29	0.39	0.14
(2,3074)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	7	0.29	0.39	0.14
(2,3074)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	7	0.29	0.39	0.14
(2,2251)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	7	0.27	0.1	0.32
(2,2251)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	7	0.27	0.1	0.32
(2,2251)	1:25:A:GLU:HB3	1:48:A:ALA:HB1	7	0.27	0.1	0.32
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	7	0.25	0.07	0.28
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	7	0.24	0.02	0.24
(2,800)	2:105:B:ALA:HB3	2:101:B:MET:HG2	7	0.23	0.09	0.21
(2,800)	2:105:B:ALA:HB3	2:101:B:MET:HG3	7	0.23	0.09	0.21
(2,800)	2:105:B:ALA:HB2	2:101:B:MET:HG2	7	0.23	0.09	0.21
(2,800)	2:105:B:ALA:HB2	2:101:B:MET:HG3	7	0.23	0.09	0.21
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	7	0.22	0.02	0.22
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	7	0.22	0.03	0.23
(2,2496)	1:51:A:LEU:HB3	1:51:A:LEU:HD22	7	0.21	0.11	0.17
(2,2496)	1:51:A:LEU:HB3	1:51:A:LEU:HD21	7	0.21	0.11	0.17
(2,2496)	1:51:A:LEU:HB2	1:51:A:LEU:HD12	7	0.21	0.11	0.17
(2,2496)	1:51:A:LEU:HB2	1:51:A:LEU:HD11	7	0.21	0.11	0.17
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	7	0.2	0.05	0.23
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	7	0.2	0.05	0.23
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB3	7	0.2	0.05	0.21
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB2	7	0.2	0.05	0.21
(2,496)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	7	0.19	0.02	0.2
(2,496)	1:25:A:GLU:HB2	1:25:A:GLU:HG3	7	0.19	0.02	0.2
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	7	0.19	0.01	0.19
(2,3234)	2:159:B:ILE:HG22	1:61:A:CYS:H	7	0.19	0.08	0.15
(2,3234)	2:159:B:ILE:HG23	1:61:A:CYS:H	7	0.19	0.08	0.15
(2,3234)	2:159:B:ILE:HG21	1:61:A:CYS:H	7	0.19	0.08	0.15
(2,3401)	1:59:A:LEU:HD11	2:159:B:ILE:HG22	7	0.19	0.04	0.19
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	7	0.19	0.04	0.19
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	7	0.19	0.04	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1678)	2:110:B:ALA:HB1	2:118:B:PRO:HA	7	0.18	0.06	0.16
(2,1678)	2:110:B:ALA:HB2	2:118:B:PRO:HA	7	0.18	0.06	0.16
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	7	0.18	0.05	0.17
(2,2057)	1:4:A:VAL:HG11	2:112:B:LEU:HB3	7	0.18	0.06	0.18
(2,2057)	1:4:A:VAL:HG13	2:112:B:LEU:HB3	7	0.18	0.06	0.18
(2,2057)	1:4:A:VAL:HG12	2:112:B:LEU:HB3	7	0.18	0.06	0.18
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	7	0.17	0.03	0.18
(2,1402)	1:26:A:ASP:HB2	1:26:A:ASP:HA	7	0.17	0.04	0.17
(2,1402)	1:26:A:ASP:HB3	1:26:A:ASP:HA	7	0.17	0.04	0.17
(2,3400)	1:59:A:LEU:HD11	2:159:B:ILE:HG22	7	0.16	0.03	0.17
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	7	0.16	0.03	0.17
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	7	0.16	0.03	0.17
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG3	7	0.14	0.03	0.14
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG2	7	0.14	0.03	0.14
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB3	7	0.14	0.03	0.14
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB2	7	0.14	0.03	0.14
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	7	0.13	0.02	0.13
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	7	0.13	0.02	0.13
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	7	0.13	0.03	0.12
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	7	0.13	0.02	0.13
(2,1392)	1:24:A:THR:HG23	1:24:A:THR:HA	7	0.13	0.01	0.13
(2,1392)	1:24:A:THR:HG22	1:24:A:THR:HA	7	0.13	0.01	0.13
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	7	0.12	0.04	0.11
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD12	7	0.12	0.02	0.12
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD13	7	0.12	0.02	0.12
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD11	7	0.12	0.02	0.12
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	7	0.12	0.0	0.12
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	7	0.11	0.01	0.11
(2,2627)	2:101:B:MET:HE1	2:102:B:ARG:H	6	0.8	0.14	0.84
(2,2627)	2:101:B:MET:HE2	2:103:B:TYR:H	6	0.8	0.14	0.84
(2,2627)	2:101:B:MET:HE3	2:104:B:VAL:H	6	0.8	0.14	0.84
(2,2627)	2:101:B:MET:HE2	2:102:B:ARG:H	6	0.8	0.14	0.84
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG2	6	0.71	0.04	0.71
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG3	6	0.71	0.04	0.71
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG2	6	0.71	0.04	0.71
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG3	6	0.71	0.04	0.71
(2,3857)	2:125:B:LYS:H	2:125:B:LYS:HE3	6	0.7	0.08	0.74
(2,792)	2:104:B:VAL:HG23	2:146:B:LEU:HD22	6	0.7	0.57	0.4
(2,792)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	6	0.7	0.57	0.4
(2,792)	2:104:B:VAL:HG22	2:146:B:LEU:HD22	6	0.7	0.57	0.4
(2,792)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	6	0.7	0.57	0.4
(2,792)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	6	0.7	0.57	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2579)	1:61:A:CYS:HB3	1:62:A:ASN:HD21	6	0.62	0.2	0.65
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD12	6	0.6	0.04	0.61
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD13	6	0.6	0.04	0.61
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.6	0.04	0.61
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD13	6	0.58	0.01	0.58
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD11	6	0.58	0.01	0.58
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD12	6	0.58	0.01	0.58
(2,2339)	1:33:A:LYS:H	1:33:A:LYS:HG3	6	0.57	0.09	0.6
(2,2337)	1:33:A:LYS:H	1:33:A:LYS:HG3	6	0.57	0.09	0.6
(2,4521)	2:145:B:GLU:HG2	2:145:B:GLU:H	6	0.53	0.15	0.48
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG22	6	0.52	0.44	0.23
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	6	0.52	0.44	0.23
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB3	6	0.45	0.21	0.44
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB2	6	0.45	0.21	0.44
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD12	6	0.45	0.02	0.44
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD13	6	0.45	0.02	0.44
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD11	6	0.45	0.02	0.44
(2,3205)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	6	0.44	0.35	0.34
(2,3205)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	6	0.44	0.35	0.34
(2,3416)	2:101:B:MET:HE1	1:17:A:HIS:HD2	6	0.43	0.07	0.43
(2,3416)	2:101:B:MET:HE2	1:17:A:HIS:HD2	6	0.43	0.07	0.43
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG3	6	0.41	0.05	0.4
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG2	6	0.41	0.05	0.4
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD12	6	0.38	0.04	0.38
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD13	6	0.38	0.04	0.38
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.38	0.04	0.38
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD12	6	0.38	0.04	0.38
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD13	6	0.38	0.04	0.38
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.38	0.04	0.38
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD12	6	0.38	0.04	0.38
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD13	6	0.38	0.04	0.38
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.38	0.04	0.38
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD12	6	0.38	0.04	0.38
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD13	6	0.38	0.04	0.38
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.38	0.04	0.38
(2,2260)	1:25:A:GLU:HG2	1:25:A:GLU:H	6	0.36	0.03	0.36
(2,2260)	1:25:A:GLU:HG3	1:25:A:GLU:H	6	0.36	0.03	0.36
(2,2808)	2:119:B:SER:HB2	2:121:B:LYS:HD3	6	0.36	0.12	0.34
(2,2808)	2:119:B:SER:HB3	2:121:B:LYS:HD3	6	0.36	0.12	0.34
(2,3355)	1:21:A:VAL:HG13	2:132:B:ILE:HB	6	0.35	0.08	0.38
(2,3355)	1:21:A:VAL:HG11	2:132:B:ILE:HB	6	0.35	0.08	0.38
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	6	0.34	0.06	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	6	0.34	0.06	0.32
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	6	0.34	0.06	0.32
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	6	0.34	0.06	0.32
(2,422)	1:15:A:ILE:HD11	2:106:B:SER:HB2	6	0.32	0.03	0.33
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	6	0.32	0.06	0.3
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	6	0.32	0.06	0.3
(2,2861)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	6	0.31	0.36	0.15
(2,329)	2:164:B:SER:H	2:162:B:LEU:HB3	6	0.29	0.12	0.3
(2,253)	2:128:B:ASP:H	2:124:B:LYS:HD2	6	0.28	0.04	0.26
(2,253)	2:128:B:ASP:H	2:125:B:LYS:HG2	6	0.28	0.04	0.26
(2,426)	1:15:A:ILE:HG21	1:18:A:ASP:HB3	6	0.28	0.13	0.23
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	6	0.28	0.06	0.26
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	6	0.28	0.06	0.26
(2,2250)	1:25:A:GLU:HB3	1:28:A:ILE:H	6	0.27	0.07	0.24
(2,2822)	2:120:B:ALA:HB3	2:140:B:ASN:H	6	0.26	0.1	0.27
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD2	6	0.25	0.12	0.21
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD3	6	0.25	0.12	0.21
(2,1962)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	6	0.24	0.05	0.23
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD13	6	0.22	0.08	0.23
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD21	6	0.22	0.08	0.23
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD23	6	0.22	0.08	0.23
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD22	6	0.22	0.08	0.23
(2,1988)	2:161:B:LYS:HD3	2:161:B:LYS:HA	6	0.2	0.02	0.22
(2,109)	1:39:A:VAL:H	1:38:A:ASN:HB3	6	0.2	0.04	0.2
(2,1967)	2:157:B:GLN:HA	2:157:B:GLN:HG2	6	0.2	0.05	0.2
(2,1866)	2:143:B:ILE:HA	2:143:B:ILE:HG12	6	0.2	0.0	0.2
(2,2142)	1:15:A:ILE:HD12	1:15:A:ILE:HA	6	0.19	0.04	0.19
(2,2142)	1:15:A:ILE:HD13	1:15:A:ILE:HA	6	0.19	0.04	0.19
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG23	6	0.18	0.03	0.19
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG22	6	0.18	0.03	0.19
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG21	6	0.18	0.03	0.19
(2,3239)	2:161:B:LYS:HD3	2:161:B:LYS:HA	6	0.17	0.02	0.18
(2,2482)	1:50:A:ALA:HB2	1:54:A:VAL:HG22	6	0.17	0.05	0.17
(2,2482)	1:50:A:ALA:HB1	1:54:A:VAL:HG12	6	0.17	0.05	0.17
(2,2482)	1:50:A:ALA:HB1	1:54:A:VAL:HG22	6	0.17	0.05	0.17
(2,2482)	1:50:A:ALA:HB3	1:54:A:VAL:HG22	6	0.17	0.05	0.17
(2,2482)	1:50:A:ALA:HB3	1:54:A:VAL:HG11	6	0.17	0.05	0.17
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB3	6	0.17	0.06	0.16
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB2	6	0.17	0.06	0.16
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB3	6	0.16	0.05	0.16
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB2	6	0.16	0.05	0.16
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG3	6	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG2	6	0.16	0.04	0.15
(2,735)	1:59:A:LEU:HA	1:59:A:LEU:HD21	6	0.15	0.03	0.15
(2,2149)	1:15:A:ILE:HD12	1:15:A:ILE:H	6	0.15	0.03	0.16
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB2	6	0.14	0.02	0.15
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB3	6	0.14	0.02	0.15
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB1	6	0.14	0.02	0.15
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB3	6	0.14	0.02	0.13
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB2	6	0.14	0.02	0.13
(2,4512)	2:143:B:ILE:HA	2:146:B:LEU:HG	6	0.13	0.02	0.13
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG21	6	0.13	0.01	0.13
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG23	6	0.13	0.01	0.13
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG12	6	0.13	0.01	0.13
(1,75)	2:126:B:ILE:N	2:122:B:ASP:O	6	0.13	0.03	0.12
(1,87)	2:142:B:VAL:N	2:138:B:ARG:O	6	0.13	0.01	0.12
(2,4136)	1:22:A:THR:HA	1:22:A:THR:HB	6	0.13	0.02	0.13
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG21	6	0.12	0.01	0.12
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG23	6	0.12	0.01	0.12
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG12	6	0.12	0.01	0.12
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	6	0.12	0.01	0.12
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	6	0.12	0.01	0.12
(2,1820)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	6	0.12	0.01	0.12
(2,1820)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	6	0.12	0.01	0.12
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB2	6	0.12	0.01	0.12
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB1	6	0.12	0.01	0.12
(2,2980)	2:134:B:ALA:HB3	2:135:B:ASP:H	6	0.11	0.02	0.11
(2,2980)	2:134:B:ALA:HB2	2:135:B:ASP:H	6	0.11	0.02	0.11
(2,2424)	1:41:A:PRO:HB3	1:41:A:PRO:HG3	6	0.1	0.0	0.1
(2,3175)	2:154:B:VAL:H	2:154:B:VAL:HG23	5	0.91	0.05	0.92
(2,181)	2:107:B:TYR:H	2:146:B:LEU:HD13	5	0.88	0.23	0.99
(2,181)	2:107:B:TYR:H	2:146:B:LEU:HD11	5	0.88	0.23	0.99
(2,3021)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	5	0.74	0.05	0.72
(2,1893)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.7	0.02	0.69
(2,2647)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	5	0.67	0.57	0.41
(2,2647)	2:104:B:VAL:HG22	2:146:B:LEU:HD22	5	0.67	0.57	0.41
(2,2647)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	5	0.67	0.57	0.41
(2,2647)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	5	0.67	0.57	0.41
(2,3103)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.66	0.02	0.65
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD22	5	0.56	0.26	0.47
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD21	5	0.56	0.26	0.47
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD13	5	0.56	0.26	0.47
(2,1134)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.54	0.02	0.53
(2,31)	1:12:A:SER:H	2:109:B:LEU:HD12	5	0.53	0.2	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,31)	1:12:A:SER:H	2:109:B:LEU:HD22	5	0.53	0.2	0.5
(2,1716)	2:121:B:LYS:HG2	2:121:B:LYS:HE2	5	0.46	0.12	0.51
(2,3050)	2:142:B:VAL:HA	2:142:B:VAL:HG21	5	0.46	0.07	0.5
(2,4458)	2:125:B:LYS:HA	2:125:B:LYS:HB3	5	0.45	0.16	0.52
(2,2921)	1:31:A:LEU:HD13	2:129:B:SER:HA	5	0.45	0.13	0.5
(2,2921)	1:31:A:LEU:HD11	2:129:B:SER:HA	5	0.45	0.13	0.5
(2,2921)	1:31:A:LEU:HD12	2:129:B:SER:HA	5	0.45	0.13	0.5
(2,1864)	2:142:B:VAL:HA	2:142:B:VAL:HG21	5	0.45	0.07	0.49
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD22	5	0.44	0.26	0.34
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD21	5	0.44	0.26	0.34
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD13	5	0.44	0.26	0.34
(2,2916)	2:128:B:ASP:HB2	2:124:B:LYS:HB3	5	0.42	0.26	0.37
(2,317)	2:154:B:VAL:H	2:154:B:VAL:HG23	5	0.41	0.05	0.43
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD13	5	0.41	0.03	0.41
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD12	5	0.41	0.03	0.41
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD11	5	0.41	0.03	0.41
(2,159)	1:63:A:VAL:H	1:62:A:ASN:HB2	5	0.41	0.16	0.35
(2,159)	1:63:A:VAL:H	1:62:A:ASN:HB3	5	0.41	0.16	0.35
(2,3055)	2:142:B:VAL:HA	2:142:B:VAL:HG21	5	0.37	0.07	0.41
(2,36)	1:13:A:ALA:H	1:51:A:LEU:HD13	5	0.33	0.23	0.24
(2,36)	1:13:A:ALA:H	1:59:A:LEU:HD11	5	0.33	0.23	0.24
(2,3493)	2:152:B:GLU:HG3	1:4:A:VAL:HB	5	0.32	0.11	0.28
(2,3493)	2:152:B:GLU:HG2	1:4:A:VAL:HB	5	0.32	0.11	0.28
(2,1085)	2:142:B:VAL:HA	2:142:B:VAL:HG21	5	0.32	0.07	0.37
(2,332)	2:165:B:VAL:H	2:164:B:SER:HB3	5	0.3	0.09	0.25
(2,332)	2:165:B:VAL:H	2:164:B:SER:HB2	5	0.3	0.09	0.25
(2,1856)	2:142:B:VAL:HA	2:142:B:VAL:HG21	5	0.3	0.07	0.35
(2,1881)	2:144:B:SER:HA	2:147:B:ASN:HB2	5	0.29	0.09	0.31
(2,1881)	2:144:B:SER:HA	2:147:B:ASN:HB3	5	0.29	0.09	0.31
(2,3178)	2:154:B:VAL:H	2:154:B:VAL:HG23	5	0.27	0.05	0.29
(2,2034)	1:2:A:ALA:HB2	1:6:A:GLU:H	5	0.27	0.11	0.23
(2,2034)	1:2:A:ALA:HB3	1:6:A:GLU:H	5	0.27	0.11	0.23
(2,1857)	2:142:B:VAL:HA	2:142:B:VAL:HG21	5	0.26	0.07	0.31
(2,1399)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	5	0.25	0.08	0.25
(2,1399)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	5	0.25	0.08	0.25
(2,1399)	1:25:A:GLU:HB3	1:48:A:ALA:HB1	5	0.25	0.08	0.25
(2,2855)	2:124:B:LYS:HA	2:124:B:LYS:HE3	5	0.25	0.04	0.27
(2,2855)	2:124:B:LYS:HA	2:124:B:LYS:HE2	5	0.25	0.04	0.27
(2,2527)	1:56:A:ILE:HD12	1:17:A:HIS:HD2	5	0.24	0.03	0.24
(2,2527)	1:56:A:ILE:HD11	1:17:A:HIS:HD2	5	0.24	0.03	0.24
(2,2527)	1:56:A:ILE:HD13	1:17:A:HIS:HD2	5	0.24	0.03	0.24
(2,1561)	1:56:A:ILE:HD11	1:10:A:ILE:HG21	5	0.23	0.03	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1561)	1:56:A:ILE:HD13	1:10:A:ILE:HG21	5	0.23	0.03	0.21
(2,1561)	1:56:A:ILE:HD12	1:10:A:ILE:HG21	5	0.23	0.03	0.21
(2,3090)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.22	0.02	0.21
(2,4520)	2:145:B:GLU:HG2	2:145:B:GLU:H	5	0.22	0.15	0.16
(2,1904)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.21	0.02	0.2
(2,660)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	5	0.21	0.05	0.2
(2,660)	1:46:A:LEU:HD22	1:42:A:PHE:HD2	5	0.21	0.05	0.2
(2,660)	1:46:A:LEU:HD22	1:42:A:PHE:HD1	5	0.21	0.05	0.2
(2,1034)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	5	0.21	0.06	0.21
(2,1418)	1:29:A:ASN:HA	1:29:A:ASN:HB3	5	0.2	0.05	0.2
(2,3303)	1:4:A:VAL:HG22	2:112:B:LEU:HD11	5	0.2	0.04	0.21
(2,3303)	1:4:A:VAL:HG12	2:112:B:LEU:HD23	5	0.2	0.04	0.21
(2,3303)	1:4:A:VAL:HG11	2:112:B:LEU:HD21	5	0.2	0.04	0.21
(2,2720)	2:110:B:ALA:H	2:110:B:ALA:HB2	5	0.18	0.04	0.19
(2,2720)	2:110:B:ALA:H	2:110:B:ALA:HB3	5	0.18	0.04	0.19
(2,2458)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	5	0.17	0.05	0.16
(2,2458)	1:46:A:LEU:HD22	1:42:A:PHE:HD2	5	0.17	0.05	0.16
(2,2458)	1:46:A:LEU:HD22	1:42:A:PHE:HD1	5	0.17	0.05	0.16
(2,719)	1:56:A:ILE:HD12	1:17:A:HIS:HD2	5	0.17	0.03	0.17
(2,719)	1:56:A:ILE:HD11	1:17:A:HIS:HD2	5	0.17	0.03	0.17
(2,719)	1:56:A:ILE:HD13	1:17:A:HIS:HD2	5	0.17	0.03	0.17
(2,851)	2:107:B:TYR:HA	2:110:B:ALA:HB2	5	0.17	0.03	0.17
(2,220)	2:119:B:SER:H	2:119:B:SER:HB3	5	0.16	0.02	0.16
(2,4251)	1:15:A:ILE:HA	2:103:B:TYR:HA	5	0.16	0.03	0.15
(2,1485)	1:39:A:VAL:HG12	1:43:A:TRP:HA	5	0.16	0.04	0.17
(2,1485)	1:39:A:VAL:HG13	1:43:A:TRP:HA	5	0.16	0.04	0.17
(2,2872)	2:125:B:LYS:HD3	2:125:B:LYS:HB2	5	0.15	0.03	0.14
(2,2872)	2:125:B:LYS:HD2	2:125:B:LYS:HB3	5	0.15	0.03	0.14
(1,81)	2:129:B:SER:N	2:125:B:LYS:O	5	0.15	0.02	0.15
(2,3011)	2:137:B:ASP:HB2	2:138:B:ARG:HG2	5	0.14	0.02	0.15
(2,3011)	2:137:B:ASP:HB3	2:138:B:ARG:HG2	5	0.14	0.02	0.15
(2,956)	2:125:B:LYS:HA	2:125:B:LYS:HG3	5	0.14	0.03	0.13
(2,956)	2:125:B:LYS:HA	2:125:B:LYS:HG2	5	0.14	0.03	0.13
(2,1567)	1:56:A:ILE:HD13	1:59:A:LEU:HG	5	0.14	0.01	0.15
(2,1567)	1:56:A:ILE:HD12	1:59:A:LEU:HG	5	0.14	0.01	0.15
(2,1567)	1:56:A:ILE:HD11	1:59:A:LEU:HG	5	0.14	0.01	0.15
(2,1757)	2:125:B:LYS:HD2	2:125:B:LYS:HG3	5	0.14	0.02	0.13
(2,1757)	2:125:B:LYS:HD3	2:125:B:LYS:HG2	5	0.14	0.02	0.13
(1,13)	1:13:A:ALA:N	1:9:A:CYS:O	5	0.13	0.02	0.12
(2,1673)	2:117:B:SER:HA	2:117:B:SER:HB2	5	0.13	0.01	0.13
(1,55)	2:107:B:TYR:N	2:103:B:TYR:O	5	0.12	0.01	0.12
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB1	5	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB3	5	0.12	0.01	0.12
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB2	5	0.12	0.01	0.12
(2,4522)	2:146:B:LEU:HA	2:146:B:LEU:HG	5	0.12	0.01	0.12
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG21	5	0.12	0.01	0.12
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG23	5	0.12	0.01	0.12
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG12	5	0.12	0.01	0.12
(2,4039)	1:46:A:LEU:HA	1:46:A:LEU:HB3	5	0.1	0.0	0.1
(2,2583)	1:61:A:CYS:HB3	1:65:A:ALA:HB3	4	1.34	0.5	1.53
(2,2583)	1:61:A:CYS:HB2	1:65:A:ALA:HB1	4	1.34	0.5	1.53
(2,385)	1:10:A:ILE:HB	1:10:A:ILE:HD11	4	0.99	0.01	0.99
(2,2096)	1:10:A:ILE:HB	1:10:A:ILE:HD11	4	0.92	0.01	0.92
(2,3336)	1:15:A:ILE:HD11	2:109:B:LEU:HD23	4	0.9	0.9	0.42
(2,3336)	1:15:A:ILE:HD13	2:109:B:LEU:HD22	4	0.9	0.9	0.42
(2,2256)	1:25:A:GLU:HG2	1:29:A:ASN:HD21	4	0.83	0.36	0.94
(2,2256)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	4	0.83	0.36	0.94
(2,3962)	2:144:B:SER:H	2:143:B:ILE:HG12	4	0.8	0.01	0.8
(2,1060)	2:139:B:LEU:HD22	2:124:B:LYS:HD2	4	0.78	0.52	0.75
(2,1060)	2:139:B:LEU:HD23	2:124:B:LYS:HD2	4	0.78	0.52	0.75
(2,384)	1:10:A:ILE:HB	1:10:A:ILE:HD11	4	0.75	0.01	0.76
(2,1809)	2:132:B:ILE:HG22	1:18:A:ASP:HB2	4	0.74	0.24	0.82
(2,1809)	2:132:B:ILE:HG23	1:18:A:ASP:HB2	4	0.74	0.24	0.82
(2,1654)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	4	0.71	0.14	0.72
(2,3017)	2:139:B:LEU:HD12	2:120:B:ALA:HA	4	0.65	0.29	0.68
(2,2088)	1:10:A:ILE:HB	1:10:A:ILE:HD11	4	0.62	0.01	0.62
(2,847)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	4	0.61	0.13	0.62
(2,1056)	2:139:B:LEU:HD22	2:124:B:LYS:HA	4	0.6	0.16	0.67
(2,1056)	2:139:B:LEU:HD12	2:120:B:ALA:HA	4	0.6	0.16	0.67
(2,1056)	2:139:B:LEU:HD21	2:124:B:LYS:HA	4	0.6	0.16	0.67
(2,1059)	2:139:B:LEU:HD12	2:120:B:ALA:HA	4	0.6	0.29	0.63
(2,242)	2:125:B:LYS:H	2:125:B:LYS:HG2	4	0.58	0.05	0.61
(2,4291)	1:26:A:ASP:HB3	1:26:A:ASP:H	4	0.56	0.01	0.56
(2,2706)	1:8:A:ALA:HA	2:109:B:LEU:HD13	4	0.54	0.57	0.27
(2,2706)	1:8:A:ALA:HA	2:109:B:LEU:HD12	4	0.54	0.57	0.27
(2,4290)	1:26:A:ASP:HB3	1:26:A:ASP:H	4	0.54	0.02	0.54
(2,2245)	1:24:A:THR:HG21	1:27:A:LYS:HE3	4	0.53	0.66	0.16
(2,2245)	1:24:A:THR:HG23	1:27:A:LYS:HE3	4	0.53	0.66	0.16
(2,846)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	4	0.47	0.14	0.48
(2,1102)	2:143:B:ILE:HD12	2:107:B:TYR:HD2	4	0.44	0.03	0.44
(2,1102)	2:143:B:ILE:HD13	2:107:B:TYR:HD2	4	0.44	0.03	0.44
(2,1017)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	4	0.44	0.2	0.5
(2,1017)	2:132:B:ILE:HG21	2:133:B:GLU:HB2	4	0.44	0.2	0.5
(2,2959)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	4	0.44	0.2	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2959)	2:132:B:ILE:HG21	2:133:B:GLU:HB2	4	0.44	0.2	0.5
(2,2965)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	4	0.44	0.2	0.5
(2,2965)	2:132:B:ILE:HG21	2:133:B:GLU:HB2	4	0.44	0.2	0.5
(2,3203)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	4	0.44	0.37	0.24
(2,3203)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	4	0.44	0.37	0.24
(2,3454)	1:35:A:ALA:HB1	2:126:B:ILE:HD13	4	0.42	0.4	0.21
(2,3454)	1:35:A:ALA:HB2	2:126:B:ILE:HD12	4	0.42	0.4	0.21
(2,3454)	1:35:A:ALA:HB1	2:126:B:ILE:HD11	4	0.42	0.4	0.21
(2,3454)	1:35:A:ALA:HB1	2:126:B:ILE:HD12	4	0.42	0.4	0.21
(2,502)	1:26:A:ASP:HB2	1:30:A:ALA:HB1	4	0.42	0.29	0.32
(2,502)	1:26:A:ASP:HB3	1:30:A:ALA:HB2	4	0.42	0.29	0.32
(2,502)	1:26:A:ASP:HB2	1:30:A:ALA:HB3	4	0.42	0.29	0.32
(2,2267)	1:26:A:ASP:HB2	1:30:A:ALA:HB1	4	0.42	0.29	0.32
(2,2267)	1:26:A:ASP:HB3	1:30:A:ALA:HB2	4	0.42	0.29	0.32
(2,2267)	1:26:A:ASP:HB2	1:30:A:ALA:HB3	4	0.42	0.29	0.32
(2,1540)	1:47:A:PHE:HA	1:51:A:LEU:HD12	4	0.42	0.35	0.25
(2,1540)	1:47:A:PHE:HA	1:51:A:LEU:HD13	4	0.42	0.35	0.25
(2,1540)	1:56:A:ILE:HA	1:51:A:LEU:HD23	4	0.42	0.35	0.25
(2,3298)	1:1:A:MET:HG3	2:153:B:ASP:HB3	4	0.41	0.14	0.36
(2,3298)	1:1:A:MET:HG3	2:153:B:ASP:HB2	4	0.41	0.14	0.36
(2,937)	2:123:B:ILE:HG21	2:106:B:SER:HA	4	0.38	0.02	0.39
(2,2849)	2:123:B:ILE:HG21	2:106:B:SER:HA	4	0.38	0.02	0.39
(2,3062)	2:142:B:VAL:HG22	2:104:B:VAL:HA	4	0.38	0.08	0.4
(2,3062)	2:142:B:VAL:HG21	2:104:B:VAL:HA	4	0.38	0.08	0.4
(2,3297)	1:1:A:MET:HE1	2:152:B:GLU:HA	4	0.37	0.14	0.42
(2,3297)	1:1:A:MET:HE2	2:152:B:GLU:HA	4	0.37	0.14	0.42
(2,3297)	1:1:A:MET:HE3	2:152:B:GLU:HA	4	0.37	0.14	0.42
(2,2850)	2:123:B:ILE:HG23	2:139:B:LEU:HA	4	0.37	0.12	0.36
(2,492)	1:25:A:GLU:HA	1:25:A:GLU:HG2	4	0.36	0.02	0.36
(2,3270)	2:165:B:VAL:HG13	2:161:B:LYS:HG3	4	0.35	0.13	0.39
(2,3270)	2:165:B:VAL:HG12	2:161:B:LYS:HG3	4	0.35	0.13	0.39
(2,3270)	2:165:B:VAL:HG12	2:161:B:LYS:HG2	4	0.35	0.13	0.39
(2,70)	1:26:A:ASP:H	1:25:A:GLU:HB2	4	0.34	0.03	0.34
(2,728)	1:54:A:VAL:HG22	1:58:A:SER:HB2	4	0.33	0.08	0.33
(2,728)	1:54:A:VAL:HG22	1:58:A:SER:HB3	4	0.33	0.08	0.33
(2,728)	1:54:A:VAL:HG21	1:58:A:SER:HB3	4	0.33	0.08	0.33
(2,728)	1:54:A:VAL:HG23	1:58:A:SER:HB2	4	0.33	0.08	0.33
(2,2588)	1:63:A:VAL:H	1:62:A:ASN:HB3	4	0.32	0.13	0.32
(2,2588)	1:63:A:VAL:H	1:62:A:ASN:HB2	4	0.32	0.13	0.32
(2,1721)	2:122:B:ASP:HA	2:125:B:LYS:HG2	4	0.32	0.12	0.29
(2,1721)	2:122:B:ASP:HA	2:125:B:LYS:HG3	4	0.32	0.12	0.29
(2,866)	2:112:B:LEU:HD12	2:108:B:LEU:HB2	4	0.32	0.07	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,866)	2:112:B:LEU:HD21	2:108:B:LEU:HB2	4	0.32	0.07	0.32
(2,707)	1:54:A:VAL:HG22	1:58:A:SER:HB2	4	0.32	0.08	0.32
(2,707)	1:54:A:VAL:HG22	1:58:A:SER:HB3	4	0.32	0.08	0.32
(2,707)	1:54:A:VAL:HG21	1:58:A:SER:HB3	4	0.32	0.08	0.32
(2,707)	1:54:A:VAL:HG23	1:58:A:SER:HB2	4	0.32	0.08	0.32
(2,2269)	1:26:A:ASP:HB3	1:27:A:LYS:H	4	0.31	0.03	0.31
(2,1885)	2:145:B:GLU:HA	2:145:B:GLU:HG2	4	0.3	0.03	0.3
(2,1314)	1:10:A:ILE:HB	1:10:A:ILE:HD11	4	0.3	0.01	0.3
(2,774)	2:101:B:MET:HE3	2:103:B:TYR:HA	4	0.3	0.11	0.26
(2,2628)	2:101:B:MET:HE3	2:103:B:TYR:HA	4	0.3	0.11	0.26
(2,497)	1:25:A:GLU:HA	1:25:A:GLU:HG2	4	0.3	0.02	0.29
(2,920)	2:122:B:ASP:HA	2:125:B:LYS:HG2	4	0.29	0.12	0.26
(2,920)	2:122:B:ASP:HA	2:125:B:LYS:HG3	4	0.29	0.12	0.26
(2,2540)	1:54:A:VAL:HG22	1:58:A:SER:HB2	4	0.27	0.08	0.27
(2,2540)	1:54:A:VAL:HG22	1:58:A:SER:HB3	4	0.27	0.08	0.27
(2,2540)	1:54:A:VAL:HG21	1:58:A:SER:HB3	4	0.27	0.08	0.27
(2,2540)	1:54:A:VAL:HG23	1:58:A:SER:HB2	4	0.27	0.08	0.27
(2,128)	1:48:A:ALA:H	1:28:A:ILE:HD12	4	0.26	0.08	0.24
(2,2261)	1:25:A:GLU:HG2	1:26:A:ASP:H	4	0.25	0.06	0.26
(2,162)	1:65:A:ALA:H	1:65:A:ALA:HB3	4	0.23	0.01	0.22
(2,162)	1:65:A:ALA:H	1:65:A:ALA:HB1	4	0.23	0.01	0.22
(2,328)	2:163:B:ALA:H	2:162:B:LEU:HB3	4	0.22	0.07	0.24
(2,169)	1:43:A:TRP:HE1	1:5:A:SER:HB2	4	0.22	0.05	0.2
(2,1373)	1:22:A:THR:HG23	1:21:A:VAL:HB	4	0.21	0.1	0.18
(2,1373)	1:22:A:THR:HG21	1:21:A:VAL:HB	4	0.21	0.1	0.18
(2,3043)	2:141:B:LYS:HA	2:144:B:SER:H	4	0.2	0.08	0.2
(2,2871)	2:125:B:LYS:H	2:125:B:LYS:HD2	4	0.19	0.06	0.22
(2,2871)	2:125:B:LYS:H	2:125:B:LYS:HD3	4	0.19	0.06	0.22
(2,1115)	2:144:B:SER:HA	2:147:B:ASN:HB2	4	0.18	0.03	0.18
(2,1115)	2:144:B:SER:HA	2:147:B:ASN:HB3	4	0.18	0.03	0.18
(2,161)	1:64:A:GLY:H	1:64:A:GLY:HA3	4	0.18	0.05	0.18
(2,161)	1:64:A:GLY:H	1:64:A:GLY:HA2	4	0.18	0.05	0.18
(2,4517)	2:144:B:SER:HA	2:143:B:ILE:HB	4	0.17	0.02	0.16
(2,1834)	2:138:B:ARG:HG2	2:138:B:ARG:HD3	4	0.16	0.04	0.16
(2,339)	1:1:A:MET:HB3	1:1:A:MET:HA	4	0.16	0.03	0.16
(2,339)	1:1:A:MET:HB2	1:1:A:MET:HA	4	0.16	0.03	0.16
(2,1574)	1:59:A:LEU:HA	1:62:A:ASN:HB3	4	0.15	0.04	0.13
(2,1574)	1:59:A:LEU:HA	1:62:A:ASN:HB2	4	0.15	0.04	0.13
(2,4393)	1:63:A:VAL:HA	1:64:A:GLY:H	4	0.14	0.04	0.12
(2,3954)	2:143:B:ILE:H	2:107:B:TYR:HE2	4	0.13	0.01	0.12
(1,32)	1:31:A:LEU:H	1:27:A:LYS:O	4	0.12	0.01	0.12
(2,1038)	2:136:B:ASP:HA	2:136:B:ASP:HB2	4	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1038)	2:136:B:ASP:HA	2:136:B:ASP:HB3	4	0.12	0.02	0.11
(2,4341)	1:41:A:PRO:HA	1:39:A:VAL:H	4	0.12	0.01	0.12
(2,3783)	2:108:B:LEU:H	2:108:B:LEU:HG	4	0.12	0.01	0.12
(2,2335)	1:33:A:LYS:HA	1:33:A:LYS:HG2	4	0.12	0.0	0.12
(2,2335)	1:33:A:LYS:HA	1:33:A:LYS:HG3	4	0.12	0.0	0.12
(2,62)	1:24:A:THR:H	1:24:A:THR:HG21	4	0.11	0.0	0.11
(2,62)	1:24:A:THR:H	1:24:A:THR:HG23	4	0.11	0.0	0.11
(2,2730)	2:108:B:LEU:HA	2:111:B:ALA:HB2	4	0.11	0.0	0.11
(2,2730)	2:108:B:LEU:HA	2:111:B:ALA:HB3	4	0.11	0.0	0.11
(1,6)	1:9:A:CYS:H	1:5:A:SER:O	4	0.11	0.01	0.11
(2,431)	1:15:A:ILE:HG23	2:105:B:ALA:HB2	4	0.11	0.01	0.11
(2,431)	1:15:A:ILE:HG23	2:105:B:ALA:HB1	4	0.11	0.01	0.11
(2,1595)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	4	0.11	0.01	0.11
(2,1765)	2:126:B:ILE:HD12	2:125:B:LYS:HD2	3	1.03	0.51	1.31
(2,1765)	2:126:B:ILE:HD12	2:125:B:LYS:HD3	3	1.03	0.51	1.31
(2,1625)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	3	0.95	0.45	1.14
(2,1625)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	3	0.95	0.45	1.14
(2,1625)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	3	0.95	0.45	1.14
(2,2645)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	3	0.94	0.45	1.13
(2,2645)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	3	0.94	0.45	1.13
(2,2645)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	3	0.94	0.45	1.13
(2,3435)	1:15:A:ILE:HD11	2:109:B:LEU:HD23	3	0.91	1.02	0.28
(2,3435)	1:15:A:ILE:HD13	2:109:B:LEU:HD22	3	0.91	1.02	0.28
(2,3435)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	3	0.91	1.02	0.28
(2,3386)	1:37:A:VAL:HG11	2:109:B:LEU:HD13	3	0.87	0.98	0.23
(2,3386)	1:37:A:VAL:HG12	2:109:B:LEU:HD13	3	0.87	0.98	0.23
(2,3386)	1:37:A:VAL:HG11	2:109:B:LEU:HD12	3	0.87	0.98	0.23
(2,3739)	1:59:A:LEU:H	1:58:A:SER:HB3	3	0.83	0.03	0.83
(2,2257)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	3	0.79	0.2	0.91
(2,790)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	3	0.78	0.45	0.97
(2,790)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	3	0.78	0.45	0.97
(2,790)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	3	0.78	0.45	0.97
(2,341)	1:1:A:MET:HG3	1:7:A:LEU:HD21	3	0.76	0.62	0.53
(2,341)	1:1:A:MET:HG2	1:7:A:LEU:HD22	3	0.76	0.62	0.53
(2,1608)	1:63:A:VAL:HA	1:63:A:VAL:HG22	3	0.74	0.03	0.76
(2,1608)	1:63:A:VAL:HA	1:63:A:VAL:HG11	3	0.74	0.03	0.76
(2,2591)	1:63:A:VAL:HA	1:63:A:VAL:HG22	3	0.7	0.03	0.71
(2,2591)	1:63:A:VAL:HA	1:63:A:VAL:HG11	3	0.7	0.03	0.71
(2,2593)	1:63:A:VAL:HA	1:63:A:VAL:HG22	3	0.63	0.04	0.65
(2,2593)	1:63:A:VAL:HA	1:63:A:VAL:HG11	3	0.63	0.04	0.65
(2,1700)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	0.59	0.18	0.58
(2,522)	1:28:A:ILE:HD12	1:44:A:PRO:HA	3	0.46	0.16	0.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1510)	1:28:A:ILE:HD12	1:44:A:PRO:HA	3	0.46	0.16	0.38
(2,2286)	1:28:A:ILE:HD12	1:44:A:PRO:HA	3	0.46	0.16	0.38
(2,3460)	1:35:A:ALA:HB1	2:126:B:ILE:HG23	3	0.44	0.11	0.37
(2,3460)	1:35:A:ALA:HB1	2:126:B:ILE:HG22	3	0.44	0.11	0.37
(2,3460)	1:35:A:ALA:HB3	2:126:B:ILE:HG21	3	0.44	0.11	0.37
(2,609)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	3	0.42	0.04	0.42
(2,609)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	3	0.42	0.04	0.42
(2,3029)	2:139:B:LEU:HD22	2:124:B:LYS:HA	3	0.4	0.05	0.43
(2,3029)	2:139:B:LEU:HD21	2:124:B:LYS:HA	3	0.4	0.05	0.43
(2,1198)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	3	0.4	0.4	0.12
(2,1198)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	3	0.4	0.4	0.12
(2,325)	2:161:B:LYS:H	2:161:B:LYS:HB2	3	0.37	0.01	0.37
(2,2748)	2:112:B:LEU:H	2:112:B:LEU:HD12	3	0.37	0.17	0.48
(2,2713)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	3	0.37	0.07	0.32
(2,1851)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	0.34	0.18	0.33
(2,2768)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	3	0.33	0.07	0.29
(2,202)	2:114:B:GLY:H	2:115:B:ASN:HB3	3	0.33	0.16	0.42
(2,1219)	2:161:B:LYS:HA	2:161:B:LYS:HG2	3	0.33	0.03	0.32
(2,1989)	2:161:B:LYS:HA	2:161:B:LYS:HG2	3	0.33	0.03	0.32
(2,2888)	1:34:A:ALA:HB1	2:126:B:ILE:HD12	3	0.32	0.1	0.27
(2,2888)	1:34:A:ALA:HB1	2:126:B:ILE:HD13	3	0.32	0.1	0.27
(2,1842)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	0.31	0.18	0.3
(2,1175)	2:154:B:VAL:HG12	2:154:B:VAL:HA	3	0.31	0.21	0.17
(2,1175)	2:154:B:VAL:HG22	2:154:B:VAL:HA	3	0.31	0.21	0.17
(2,1946)	2:154:B:VAL:HG22	2:149:B:LYS:HG2	3	0.3	0.06	0.31
(2,1946)	2:154:B:VAL:HG23	2:149:B:LYS:HG2	3	0.3	0.06	0.31
(2,1946)	2:154:B:VAL:HG22	2:149:B:LYS:HG3	3	0.3	0.06	0.31
(2,2717)	2:110:B:ALA:HB1	2:115:B:ASN:HD21	3	0.3	0.02	0.28
(2,2717)	2:110:B:ALA:HB2	2:115:B:ASN:HD21	3	0.3	0.02	0.28
(2,3237)	2:161:B:LYS:HA	2:161:B:LYS:HG2	3	0.3	0.03	0.29
(2,327)	2:162:B:LEU:H	2:162:B:LEU:HB2	3	0.29	0.02	0.3
(2,3247)	2:162:B:LEU:H	2:162:B:LEU:HB2	3	0.29	0.02	0.3
(2,1090)	2:142:B:VAL:HG22	2:146:B:LEU:HD22	3	0.29	0.1	0.35
(2,1090)	2:142:B:VAL:HG22	2:146:B:LEU:HD23	3	0.29	0.1	0.35
(2,12)	1:3:A:SER:H	1:6:A:GLU:HG2	3	0.29	0.06	0.3
(2,2723)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	3	0.29	0.07	0.25
(2,761)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	0.28	0.12	0.26
(2,1307)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	3	0.28	0.04	0.28
(2,1307)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	3	0.28	0.04	0.28
(2,875)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	3	0.28	0.07	0.24
(2,3168)	2:154:B:VAL:HG12	2:154:B:VAL:HA	3	0.28	0.21	0.14
(2,3168)	2:154:B:VAL:HG22	2:154:B:VAL:HA	3	0.28	0.21	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,334)	2:167:B:ALA:H	2:167:B:ALA:HB3	3	0.27	0.12	0.23
(2,334)	2:167:B:ALA:H	2:167:B:ALA:HB2	3	0.27	0.12	0.23
(2,434)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	3	0.26	0.06	0.24
(2,2405)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	3	0.24	0.04	0.24
(2,2405)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	3	0.24	0.04	0.24
(2,279)	2:139:B:LEU:H	2:139:B:LEU:HD13	3	0.24	0.07	0.2
(2,2165)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	3	0.22	0.06	0.19
(2,3256)	2:162:B:LEU:HD11	2:159:B:ILE:HA	3	0.22	0.09	0.15
(2,3256)	2:162:B:LEU:HD13	2:159:B:ILE:HA	3	0.22	0.09	0.15
(2,704)	1:54:A:VAL:HG22	1:58:A:SER:HB2	3	0.21	0.05	0.21
(2,704)	1:54:A:VAL:HG22	1:58:A:SER:HB3	3	0.21	0.05	0.21
(2,704)	1:54:A:VAL:HG21	1:58:A:SER:HB3	3	0.21	0.05	0.21
(2,1792)	2:130:B:VAL:HG22	2:127:B:LEU:HA	3	0.21	0.03	0.22
(2,3013)	2:139:B:LEU:H	2:139:B:LEU:HD13	3	0.21	0.07	0.17
(2,2285)	1:28:A:ILE:HA	1:31:A:LEU:HD22	3	0.2	0.06	0.17
(2,3004)	2:138:B:ARG:HB3	2:138:B:ARG:HD2	3	0.2	0.07	0.19
(2,3378)	1:35:A:ALA:HB1	2:126:B:ILE:HD13	3	0.2	0.02	0.19
(2,3378)	1:35:A:ALA:HB1	2:126:B:ILE:HD11	3	0.2	0.02	0.19
(2,3378)	1:35:A:ALA:HB1	2:126:B:ILE:HD12	3	0.2	0.02	0.19
(2,2992)	2:137:B:ASP:HA	2:140:B:ASN:HB3	3	0.19	0.04	0.2
(2,1641)	2:108:B:LEU:HD21	2:155:B:ILE:HG21	3	0.19	0.1	0.15
(2,3413)	2:101:B:MET:HE2	1:14:A:LEU:HB2	3	0.19	0.08	0.16
(2,3413)	2:101:B:MET:HE1	1:14:A:LEU:HB2	3	0.19	0.08	0.16
(2,1465)	1:37:A:VAL:HG22	1:4:A:VAL:HG11	3	0.19	0.04	0.21
(2,1465)	1:37:A:VAL:HG23	1:4:A:VAL:HG11	3	0.19	0.04	0.21
(2,615)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	3	0.18	0.04	0.18
(2,615)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	3	0.18	0.04	0.18
(2,1075)	2:142:B:VAL:HA	2:142:B:VAL:HG21	3	0.18	0.0	0.18
(2,316)	2:154:B:VAL:H	2:154:B:VAL:HG23	3	0.17	0.02	0.18
(2,671)	1:49:A:LYS:HA	1:49:A:LYS:HD2	3	0.17	0.05	0.2
(2,1076)	2:142:B:VAL:HA	2:142:B:VAL:HG21	3	0.17	0.0	0.17
(2,3238)	2:161:B:LYS:H	2:161:B:LYS:HB2	3	0.16	0.01	0.16
(2,299)	2:146:B:LEU:H	2:146:B:LEU:HD22	3	0.16	0.02	0.15
(2,1995)	2:162:B:LEU:HA	2:162:B:LEU:HB3	3	0.16	0.02	0.16
(2,3079)	2:143:B:ILE:HA	2:143:B:ILE:HG21	3	0.16	0.0	0.16
(2,3044)	2:142:B:VAL:HA	2:142:B:VAL:HG21	3	0.15	0.0	0.15
(2,3308)	1:4:A:VAL:HG22	2:112:B:LEU:HD11	3	0.15	0.01	0.15
(2,3308)	1:4:A:VAL:HG11	2:112:B:LEU:HD21	3	0.15	0.01	0.15
(2,3308)	1:4:A:VAL:HG12	2:112:B:LEU:HD23	3	0.15	0.01	0.15
(2,670)	1:49:A:LYS:HA	1:49:A:LYS:HB3	3	0.14	0.01	0.15
(2,670)	1:49:A:LYS:HA	1:49:A:LYS:HB2	3	0.14	0.01	0.15
(2,1665)	1:4:A:VAL:HB	2:112:B:LEU:HD22	3	0.14	0.02	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1665)	1:4:A:VAL:HB	2:112:B:LEU:HD21	3	0.14	0.02	0.15
(2,1665)	1:4:A:VAL:HB	2:112:B:LEU:HD23	3	0.14	0.02	0.15
(2,3302)	1:4:A:VAL:HB	2:112:B:LEU:HD22	3	0.14	0.02	0.15
(2,3302)	1:4:A:VAL:HB	2:112:B:LEU:HD21	3	0.14	0.02	0.15
(2,3302)	1:4:A:VAL:HB	2:112:B:LEU:HD23	3	0.14	0.02	0.15
(2,500)	1:26:A:ASP:HA	1:29:A:ASN:HB2	3	0.14	0.04	0.13
(2,500)	1:26:A:ASP:HA	1:29:A:ASN:HB3	3	0.14	0.04	0.13
(2,1545)	1:53:A:ASN:HA	1:53:A:ASN:HB2	3	0.14	0.01	0.14
(2,1545)	1:53:A:ASN:HA	1:53:A:ASN:HB3	3	0.14	0.01	0.14
(2,4446)	2:120:B:ALA:HA	2:140:B:ASN:HA	3	0.14	0.02	0.13
(2,3528)	1:5:A:SER:H	1:3:A:SER:HA	3	0.13	0.03	0.13
(2,383)	1:10:A:ILE:HA	1:13:A:ALA:HB1	3	0.13	0.03	0.11
(2,383)	1:10:A:ILE:HA	1:13:A:ALA:HB2	3	0.13	0.03	0.11
(2,208)	2:115:B:ASN:H	2:111:B:ALA:HB3	3	0.13	0.02	0.11
(2,2045)	1:4:A:VAL:HA	1:7:A:LEU:HD21	3	0.13	0.02	0.13
(2,2727)	2:115:B:ASN:H	2:111:B:ALA:HB3	3	0.13	0.02	0.11
(2,214)	2:117:B:SER:H	2:117:B:SER:HB3	3	0.12	0.02	0.12
(2,1370)	1:19:A:ASP:HB3	1:21:A:VAL:HG13	3	0.12	0.02	0.11
(2,1370)	1:19:A:ASP:HB3	1:21:A:VAL:HG12	3	0.12	0.02	0.11
(2,3728)	1:55:A:ASN:H	1:54:A:VAL:H	3	0.12	0.02	0.13
(2,267)	2:134:B:ALA:H	2:133:B:GLU:HB3	3	0.12	0.01	0.11
(2,566)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	3	0.12	0.01	0.11
(2,566)	1:34:A:ALA:HB3	2:126:B:ILE:HG13	3	0.12	0.01	0.11
(2,1709)	2:121:B:LYS:HA	2:121:B:LYS:HD2	3	0.12	0.01	0.12
(2,2345)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	3	0.12	0.01	0.11
(2,2345)	1:34:A:ALA:HB3	2:126:B:ILE:HG13	3	0.12	0.01	0.11
(2,3371)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	3	0.12	0.01	0.11
(2,3371)	1:34:A:ALA:HB3	2:126:B:ILE:HG13	3	0.12	0.01	0.11
(2,4046)	1:56:A:ILE:HG12	1:56:A:ILE:HA	3	0.12	0.01	0.12
(2,2229)	1:23:A:VAL:HG22	1:16:A:LEU:HG	3	0.12	0.02	0.11
(2,2229)	1:23:A:VAL:HG21	1:16:A:LEU:HG	3	0.12	0.02	0.11
(2,2259)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	3	0.12	0.0	0.12
(2,1361)	1:20:A:GLU:HA	1:20:A:GLU:HG2	3	0.11	0.01	0.11
(2,1021)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	3	0.11	0.0	0.11
(2,1021)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	3	0.11	0.0	0.11
(1,73)	2:125:B:LYS:N	2:121:B:LYS:O	3	0.11	0.01	0.11
(2,1870)	2:143:B:ILE:HD11	2:143:B:ILE:HG12	3	0.11	0.0	0.11
(2,1870)	2:143:B:ILE:HD11	2:143:B:ILE:HG13	3	0.11	0.0	0.11
(2,2082)	1:8:A:ALA:HB3	1:5:A:SER:HA	3	0.11	0.0	0.11
(2,1999)	2:162:B:LEU:HA	2:162:B:LEU:HD13	3	0.1	0.0	0.1
(2,1999)	2:162:B:LEU:HA	2:162:B:LEU:HD11	3	0.1	0.0	0.1
(2,3269)	2:165:B:VAL:H	2:165:B:VAL:HG22	2	1.02	0.86	1.02

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,3269)	2:165:B:VAL:H	2:165:B:VAL:HG21	2	1.02	0.86	1.02
(2,1242)	2:165:B:VAL:HG13	2:166:B:PRO:HD2	2	0.97	0.79	0.97
(2,1242)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	2	0.97	0.79	0.97
(2,950)	2:125:B:LYS:HB2	2:122:B:ASP:HB3	2	0.94	0.09	0.94
(2,1243)	2:165:B:VAL:HG13	2:166:B:PRO:HD2	2	0.9	0.79	0.9
(2,1243)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	2	0.9	0.79	0.9
(2,3274)	2:165:B:VAL:HG13	2:166:B:PRO:HD2	2	0.9	0.78	0.9
(2,3274)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	2	0.9	0.78	0.9
(2,4008)	1:4:A:VAL:HB	1:3:A:SER:HB3	2	0.8	0.01	0.8
(2,4222)	1:4:A:VAL:HB	1:3:A:SER:HB3	2	0.8	0.01	0.8
(2,3390)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	2	0.78	0.08	0.78
(2,836)	1:8:A:ALA:HA	2:109:B:LEU:HD12	2	0.78	0.57	0.78
(2,836)	1:8:A:ALA:HA	2:109:B:LEU:HD13	2	0.78	0.57	0.78
(2,3267)	2:165:B:VAL:HA	2:165:B:VAL:HG22	2	0.76	0.52	0.76
(2,3267)	2:165:B:VAL:HA	2:165:B:VAL:HG12	2	0.76	0.52	0.76
(2,1238)	2:165:B:VAL:HA	2:165:B:VAL:HG22	2	0.72	0.52	0.72
(2,1238)	2:165:B:VAL:HA	2:165:B:VAL:HG12	2	0.72	0.52	0.72
(2,2013)	2:165:B:VAL:HA	2:165:B:VAL:HG22	2	0.7	0.52	0.7
(2,2013)	2:165:B:VAL:HA	2:165:B:VAL:HG12	2	0.7	0.52	0.7
(2,3166)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	2	0.7	0.1	0.7
(2,438)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	2	0.68	0.11	0.68
(2,117)	1:43:A:TRP:H	1:40:A:GLU:HG2	2	0.63	0.01	0.63
(2,2169)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	2	0.63	0.11	0.63
(2,1849)	2:139:B:LEU:HD22	2:124:B:LYS:HD2	2	0.62	0.26	0.62
(2,1849)	2:139:B:LEU:HD23	2:124:B:LYS:HD2	2	0.62	0.26	0.62
(2,2373)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	2	0.62	0.07	0.62
(2,1746)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	2	0.57	0.46	0.57
(2,4080)	2:122:B:ASP:HA	2:125:B:LYS:HB2	2	0.57	0.07	0.57
(2,586)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	2	0.56	0.07	0.56
(2,4462)	2:125:B:LYS:H	2:125:B:LYS:HB2	2	0.54	0.05	0.54
(2,3385)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	2	0.52	0.07	0.52
(2,1824)	2:134:B:ALA:HB3	2:124:B:LYS:HE2	2	0.52	0.42	0.52
(2,4084)	2:124:B:LYS:HA	2:124:B:LYS:HD2	2	0.49	0.32	0.49
(2,1383)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	2	0.48	0.12	0.48
(2,217)	2:117:B:SER:H	2:115:B:ASN:HD21	2	0.48	0.01	0.48
(2,621)	1:40:A:GLU:HG3	1:42:A:PHE:HE1	2	0.43	0.02	0.43
(2,3131)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	2	0.43	0.1	0.43
(2,4456)	2:124:B:LYS:HA	2:124:B:LYS:HD2	2	0.42	0.22	0.42
(2,337)	2:169:B:GLY:H	2:168:B:GLY:HA3	2	0.42	0.04	0.42
(2,1351)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	2	0.42	0.11	0.42
(2,2410)	1:40:A:GLU:HG3	1:42:A:PHE:HE1	2	0.42	0.02	0.42
(2,189)	2:112:B:LEU:H	2:112:B:LEU:HD12	2	0.4	0.02	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,136)	1:51:A:LEU:H	1:50:A:ALA:HB2	2	0.38	0.03	0.38
(2,772)	2:101:B:MET:HE3	2:105:B:ALA:HB2	2	0.38	0.01	0.38
(2,3858)	2:125:B:LYS:H	2:125:B:LYS:HB2	2	0.38	0.05	0.38
(2,414)	1:14:A:LEU:HD12	2:101:B:MET:HG3	2	0.37	0.04	0.37
(2,637)	1:42:A:PHE:HB3	1:42:A:PHE:HD2	2	0.36	0.01	0.36
(2,1384)	1:23:A:VAL:HG12	1:51:A:LEU:HD13	2	0.34	0.01	0.34
(2,1384)	1:23:A:VAL:HG13	1:51:A:LEU:HD22	2	0.34	0.01	0.34
(2,1041)	2:137:B:ASP:HA	2:141:B:LYS:HB2	2	0.33	0.09	0.33
(2,1829)	2:137:B:ASP:HA	2:141:B:LYS:HB2	2	0.33	0.09	0.33
(2,2991)	2:137:B:ASP:HA	2:141:B:LYS:HB2	2	0.33	0.09	0.33
(2,3445)	2:112:B:LEU:HA	1:37:A:VAL:HG21	2	0.33	0.04	0.33
(2,3162)	2:154:B:VAL:HG12	2:154:B:VAL:HA	2	0.32	0.22	0.32
(2,3162)	2:154:B:VAL:HG22	2:154:B:VAL:HA	2	0.32	0.22	0.32
(2,3340)	1:15:A:ILE:HD11	2:127:B:LEU:HB3	2	0.31	0.18	0.31
(2,4181)	2:124:B:LYS:HA	2:124:B:LYS:HD2	2	0.3	0.01	0.3
(2,2431)	1:42:A:PHE:HB3	1:42:A:PHE:HD2	2	0.29	0.0	0.29
(2,3109)	2:104:B:VAL:HG21	2:146:B:LEU:HD22	2	0.27	0.02	0.27
(2,3109)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	2	0.27	0.02	0.27
(2,3469)	2:130:B:VAL:HG21	1:16:A:LEU:HB2	2	0.27	0.04	0.27
(2,1142)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	2	0.26	0.09	0.26
(2,4391)	1:61:A:CYS:HA	1:62:A:ASN:HA	2	0.26	0.01	0.26
(2,2972)	2:134:B:ALA:HB2	2:139:B:LEU:HD22	2	0.26	0.1	0.26
(2,2972)	2:134:B:ALA:HB3	2:139:B:LEU:HD22	2	0.26	0.1	0.26
(2,3332)	1:14:A:LEU:HD12	2:101:B:MET:HG3	2	0.26	0.03	0.26
(2,775)	1:14:A:LEU:HD12	2:101:B:MET:HE1	2	0.24	0.0	0.24
(2,775)	1:14:A:LEU:HD12	2:101:B:MET:HE2	2	0.24	0.0	0.24
(2,195)	2:113:B:GLY:H	2:112:B:LEU:HD23	2	0.22	0.02	0.22
(2,195)	2:113:B:GLY:H	2:112:B:LEU:HD22	2	0.22	0.02	0.22
(2,1033)	2:134:B:ALA:HB2	2:139:B:LEU:HD22	2	0.22	0.11	0.22
(2,1033)	2:134:B:ALA:HB3	2:139:B:LEU:HD22	2	0.22	0.11	0.22
(2,3334)	1:14:A:LEU:HD11	2:162:B:LEU:HD22	2	0.22	0.01	0.22
(2,3334)	1:14:A:LEU:HD12	2:162:B:LEU:HD22	2	0.22	0.01	0.22
(2,2860)	2:124:B:LYS:HG2	2:124:B:LYS:HE3	2	0.22	0.08	0.22
(2,2860)	2:124:B:LYS:HG3	2:124:B:LYS:HE2	2	0.22	0.08	0.22
(2,2625)	2:101:B:MET:HE3	2:105:B:ALA:HB2	2	0.21	0.01	0.21
(2,3494)	1:7:A:LEU:HD13	2:155:B:ILE:HG22	2	0.21	0.08	0.21
(2,3494)	1:7:A:LEU:HD12	2:155:B:ILE:HG23	2	0.21	0.08	0.21
(2,2949)	2:132:B:ILE:HD11	2:132:B:ILE:H	2	0.2	0.02	0.2
(2,3377)	1:34:A:ALA:HB2	2:126:B:ILE:HB	2	0.2	0.03	0.2
(2,2601)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	2	0.2	0.08	0.2
(2,199)	2:114:B:GLY:H	2:112:B:LEU:H	2	0.2	0.01	0.2
(2,673)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	2	0.19	0.02	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2255)	1:25:A:GLU:HG2	1:26:A:ASP:HA	2	0.18	0.02	0.18
(2,4360)	1:52:A:ALA:HA	1:23:A:VAL:HG13	2	0.18	0.08	0.18
(2,340)	1:1:A:MET:HG2	1:1:A:MET:HB2	2	0.18	0.0	0.18
(2,340)	1:1:A:MET:HG3	1:1:A:MET:HB2	2	0.18	0.0	0.18
(2,427)	1:15:A:ILE:HG22	2:127:B:LEU:HG	2	0.18	0.06	0.18
(2,2130)	1:14:A:LEU:HD12	2:101:B:MET:HG3	2	0.18	0.04	0.18
(2,763)	1:43:A:TRP:HD1	1:6:A:GLU:HG3	2	0.18	0.0	0.18
(2,1931)	2:152:B:GLU:HA	2:152:B:GLU:HB3	2	0.17	0.06	0.17
(2,1093)	2:143:B:ILE:HA	2:146:B:LEU:HD13	2	0.17	0.02	0.17
(2,20)	1:8:A:ALA:H	1:7:A:LEU:HD22	2	0.16	0.04	0.16
(2,20)	1:8:A:ALA:H	1:7:A:LEU:HD21	2	0.16	0.04	0.16
(2,196)	2:113:B:GLY:H	1:37:A:VAL:HG11	2	0.16	0.02	0.16
(2,196)	2:113:B:GLY:H	1:37:A:VAL:HG13	2	0.16	0.02	0.16
(2,1814)	2:133:B:GLU:HA	2:133:B:GLU:HG2	2	0.16	0.04	0.16
(2,2511)	1:54:A:VAL:HG22	1:58:A:SER:HB2	2	0.16	0.03	0.16
(2,2511)	1:54:A:VAL:HG22	1:58:A:SER:HB3	2	0.16	0.03	0.16
(2,1084)	2:103:B:TYR:HB2	2:142:B:VAL:HG11	2	0.16	0.02	0.16
(2,1084)	2:103:B:TYR:HB2	2:142:B:VAL:HG13	2	0.16	0.02	0.16
(2,2478)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	2	0.16	0.02	0.16
(2,3489)	2:152:B:GLU:HG3	1:7:A:LEU:HG	2	0.16	0.04	0.16
(2,4524)	2:146:B:LEU:H	2:146:B:LEU:HG	2	0.16	0.01	0.16
(1,67)	2:113:B:GLY:N	2:109:B:LEU:O	2	0.15	0.0	0.15
(1,68)	2:113:B:GLY:H	2:109:B:LEU:O	2	0.15	0.0	0.15
(2,2398)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	2	0.15	0.03	0.15
(2,2398)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	2	0.15	0.03	0.15
(2,2654)	2:105:B:ALA:HB3	2:162:B:LEU:HD23	2	0.15	0.03	0.15
(1,25)	1:28:A:ILE:N	1:24:A:THR:O	2	0.15	0.0	0.15
(2,157)	1:62:A:ASN:H	1:62:A:ASN:HB3	2	0.14	0.01	0.14
(2,304)	2:149:B:LYS:H	2:149:B:LYS:HE2	2	0.14	0.01	0.14
(2,773)	2:101:B:MET:HE2	2:101:B:MET:HG3	2	0.14	0.03	0.14
(2,773)	2:101:B:MET:HE3	2:101:B:MET:HG2	2	0.14	0.03	0.14
(2,2590)	1:62:A:ASN:H	1:62:A:ASN:HB3	2	0.14	0.01	0.14
(2,3085)	2:144:B:SER:H	2:144:B:SER:HB2	2	0.14	0.01	0.14
(2,4001)	2:164:B:SER:H	2:163:B:ALA:HA	2	0.14	0.01	0.14
(1,91)	2:144:B:SER:N	2:140:B:ASN:O	2	0.13	0.01	0.13
(2,1530)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	2	0.13	0.02	0.13
(2,2602)	1:43:A:TRP:HD1	1:6:A:GLU:HG3	2	0.13	0.0	0.13
(2,599)	1:39:A:VAL:HA	1:39:A:VAL:HG11	2	0.12	0.01	0.12
(2,599)	1:39:A:VAL:HA	1:39:A:VAL:HG13	2	0.12	0.01	0.12
(2,786)	2:104:B:VAL:HA	2:107:B:TYR:HD2	2	0.12	0.01	0.12
(2,786)	2:104:B:VAL:HA	2:107:B:TYR:HD1	2	0.12	0.01	0.12
(2,2629)	1:14:A:LEU:HD12	2:101:B:MET:HE1	2	0.12	0.01	0.12

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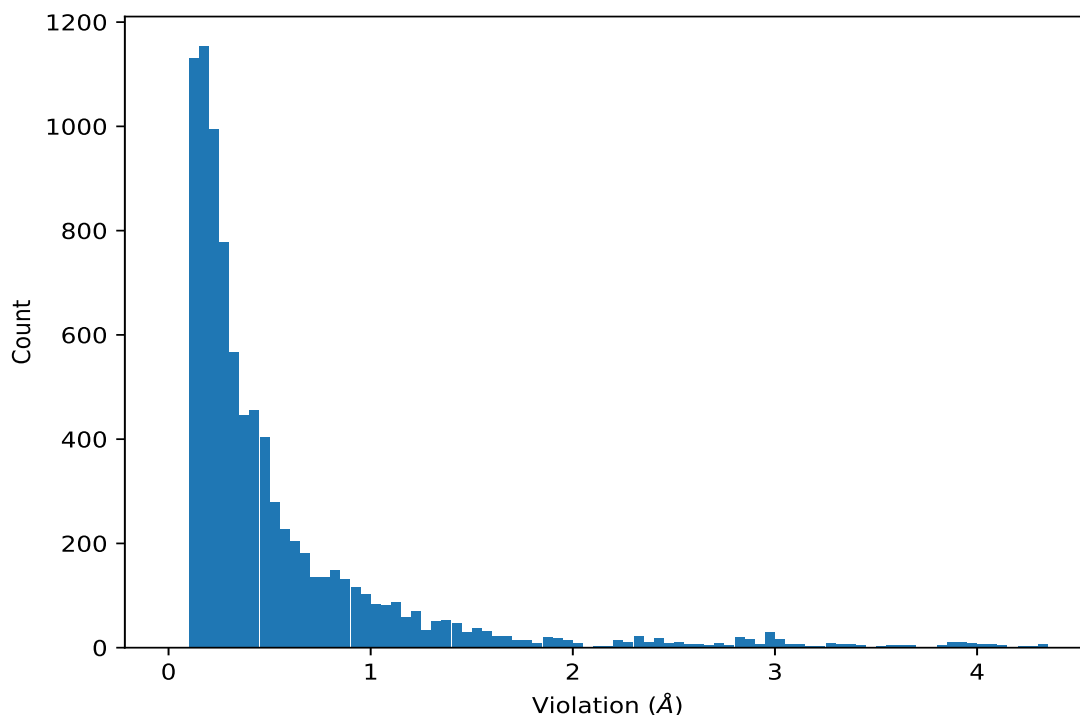
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2629)	1:14:A:LEU:HD12	2:101:B:MET:HE2	2	0.12	0.01	0.12
(1,99)	2:155:B:ILE:N	2:151:B:ILE:O	2	0.12	0.0	0.12
(2,72)	1:27:A:LYS:H	1:28:A:ILE:HD11	2	0.12	0.0	0.12
(2,1556)	1:55:A:ASN:HA	1:55:A:ASN:HB2	2	0.12	0.0	0.12
(2,3236)	2:161:B:LYS:HA	2:161:B:LYS:HB3	2	0.12	0.01	0.12
(2,1135)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	2	0.12	0.02	0.12
(2,1968)	2:157:B:GLN:HA	2:157:B:GLN:HB3	2	0.12	0.02	0.12
(2,2559)	1:59:A:LEU:HA	1:59:A:LEU:HD21	2	0.12	0.0	0.12
(2,3211)	2:157:B:GLN:H	2:157:B:GLN:HG2	2	0.12	0.0	0.12
(2,3736)	1:58:A:SER:H	1:55:A:ASN:HA	2	0.12	0.0	0.12
(2,852)	2:110:B:ALA:HA	2:110:B:ALA:HB3	2	0.11	0.01	0.11
(2,1100)	2:143:B:ILE:HD13	2:123:B:ILE:HA	2	0.11	0.0	0.11
(2,1100)	2:143:B:ILE:HD11	2:123:B:ILE:HA	2	0.11	0.0	0.11
(2,2084)	1:39:A:VAL:HG21	1:9:A:CYS:HA	2	0.11	0.0	0.11
(2,3139)	2:151:B:ILE:HB	2:151:B:ILE:HD13	2	0.11	0.01	0.11
(2,3745)	1:61:A:CYS:H	1:62:A:ASN:HA	2	0.11	0.0	0.11
(1,56)	2:107:B:TYR:H	2:103:B:TYR:O	2	0.11	0.0	0.11
(2,612)	1:39:A:VAL:HA	1:39:A:VAL:HG11	2	0.11	0.0	0.11
(2,612)	1:39:A:VAL:HA	1:39:A:VAL:HG13	2	0.11	0.0	0.11
(2,1587)	1:59:A:LEU:HA	1:59:A:LEU:HD21	2	0.11	0.0	0.11
(2,2419)	1:41:A:PRO:HA	1:41:A:PRO:HG3	2	0.11	0.0	0.11
(2,3052)	2:103:B:TYR:HB2	2:142:B:VAL:HG12	2	0.11	0.0	0.11
(2,3052)	2:103:B:TYR:HB2	2:142:B:VAL:HG11	2	0.11	0.0	0.11
(2,3141)	2:151:B:ILE:HA	2:151:B:ILE:HD11	2	0.11	0.0	0.11
(2,705)	1:54:A:VAL:HA	1:54:A:VAL:HG12	2	0.1	0.0	0.1
(2,705)	1:54:A:VAL:HA	1:54:A:VAL:HG13	2	0.1	0.0	0.1

<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)
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	6	4.33
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	9	4.33
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	8	4.32
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	2	4.3
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	4	4.3
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	5	4.3
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	10	4.28
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	3	4.27
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	7	4.24
(2,4060)	1:11:A:TYR:HE1	2:112:B:LEU:HG	1	4.21
(2,3505)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	1	4.13
(2,1215)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	1	4.13
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	6	4.12
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	9	4.11
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	8	4.1
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	2	4.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	4	4.09
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	5	4.09
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	10	4.07
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	3	4.06
(2,3505)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	6	4.06
(2,1215)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	6	4.06
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	7	4.03
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	10	4.03
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	8	4.02
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	1	4.01
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	4	4.01
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	7	4.01
(2,4402)	1:11:A:TYR:HE1	2:112:B:LEU:HG	1	4.0
(2,3505)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	7	3.99
(2,1215)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	7	3.99
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	5	3.98
(2,3505)	2:159:B:ILE:HG21	1:11:A:TYR:HE2	4	3.95
(2,3505)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	8	3.95
(2,3505)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	10	3.95
(2,1215)	2:159:B:ILE:HG21	1:11:A:TYR:HE2	4	3.95
(2,1215)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	8	3.95
(2,1215)	2:159:B:ILE:HG23	1:11:A:TYR:HE2	10	3.95
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	10	3.94
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	8	3.93
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	1	3.92
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	4	3.92
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	7	3.92
(2,3505)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	2	3.92
(2,1215)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	2	3.92
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	2	3.91
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	3	3.91
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	6	3.9
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	9	3.89
(2,4249)	1:14:A:LEU:HG	1:11:A:TYR:HD2	9	3.89
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	9	3.89
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	5	3.89
(2,3505)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	3	3.89
(2,3505)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	9	3.89
(2,1215)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	3	3.89
(2,1215)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	9	3.89
(2,3505)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	5	3.85
(2,1215)	2:159:B:ILE:HG22	1:11:A:TYR:HE2	5	3.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	2	3.82
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	3	3.82
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	6	3.81
(2,4016)	1:14:A:LEU:HG	1:11:A:TYR:HD2	9	3.8
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	8	3.69
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	8	3.69
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	5	3.68
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	5	3.68
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	2	3.64
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	2	3.64
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	6	3.61
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	6	3.61
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	7	3.57
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	7	3.57
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	4	3.55
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	4	3.55
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	1	3.53
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	1	3.53
(2,869)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	2	3.44
(2,869)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	4	3.42
(2,869)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	5	3.42
(2,695)	1:51:A:LEU:HD11	1:48:A:ALA:HA	6	3.42
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	3	3.39
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	6	3.39
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	3	3.39
(2,2909)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	10	3.39
(2,2462)	1:47:A:PHE:HB2	1:59:A:LEU:HD13	6	3.39
(2,978)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	10	3.39
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	8	3.35
(2,4496)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	10	3.34
(2,4096)	2:138:B:ARG:HD3	2:103:B:TYR:HE1	10	3.34
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	1	3.33
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	7	3.33
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	4	3.31
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	10	3.3
(2,3449)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	2	3.3
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	2	3.29
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	3	3.29
(2,3449)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	4	3.28
(2,3449)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	5	3.28
(2,2740)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	2	3.28
(2,2740)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	4	3.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2740)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	5	3.26
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	5	3.25
(2,869)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	1	3.24
(2,2905)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	10	3.22
(2,977)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	10	3.22
(2,4401)	1:11:A:TYR:HE2	2:159:B:ILE:HA	9	3.19
(2,869)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	3	3.18
(2,869)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	7	3.11
(2,869)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	10	3.11
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	6	3.1
(2,3449)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	1	3.1
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	6	3.1
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	6	3.1
(2,2740)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	1	3.08
(2,2909)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	5	3.07
(2,2905)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	5	3.07
(2,978)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	5	3.07
(2,977)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	5	3.07
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	9	3.06
(2,869)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	9	3.05
(2,3449)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	3	3.04
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	9	3.04
(2,799)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	8	3.04
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	1	3.02
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	1	3.02
(2,2740)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	3	3.02
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	1	3.02
(2,2909)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	2	3.01
(2,2905)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	6	3.01
(2,978)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	2	3.01
(2,977)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	6	3.01
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	8	3.01
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	3.01
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	4	3.0
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	4	3.0
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	4	3.0
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	7	2.99
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	7	2.99
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	8	2.99
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	7	2.99
(2,869)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	8	2.99
(2,799)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	6	2.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	5	2.99
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	10	2.98
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	10	2.98
(2,2909)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	6	2.98
(2,2909)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	7	2.98
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	2.98
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	10	2.98
(2,978)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	6	2.98
(2,978)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	7	2.98
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	3	2.98
(2,799)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	5	2.98
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	5	2.97
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	3	2.97
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	4	2.97
(2,3449)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	7	2.96
(2,3449)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	10	2.96
(2,2909)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	1	2.96
(2,978)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	1	2.96
(2,869)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	6	2.96
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	2	2.96
(2,2740)	2:112:B:LEU:HD12	1:11:A:TYR:HE1	7	2.95
(2,2740)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	10	2.95
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	3	2.95
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	4	2.95
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	2	2.94
(2,1542)	1:51:A:LEU:HD21	1:56:A:ILE:HB	6	2.92
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	6	2.92
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	7	2.92
(2,3449)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	9	2.91
(2,2905)	2:127:B:LEU:HD21	2:103:B:TYR:HD2	3	2.91
(2,977)	2:127:B:LEU:HD21	2:103:B:TYR:HD2	3	2.91
(2,2740)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	9	2.89
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	6	2.89
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	7	2.89
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	2	2.88
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	9	2.88
(2,2905)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	2	2.87
(2,2905)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	4	2.87
(2,977)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	2	2.87
(2,977)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	4	2.87
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	7	2.87
(2,2905)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	1	2.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2905)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	7	2.85
(2,977)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	1	2.85
(2,977)	2:127:B:LEU:HD22	2:103:B:TYR:HD2	7	2.85
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	1	2.85
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	10	2.85
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	9	2.84
(2,3449)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	8	2.84
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	9	2.84
(2,2905)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	9	2.84
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	9	2.84
(2,977)	2:127:B:LEU:HD23	2:103:B:TYR:HD2	9	2.84
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	1	2.83
(2,2905)	2:127:B:LEU:HD21	2:103:B:TYR:HD2	8	2.83
(2,2740)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	8	2.83
(2,977)	2:127:B:LEU:HD21	2:103:B:TYR:HD2	8	2.83
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	4	2.82
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	5	2.82
(2,3449)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	6	2.81
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	8	2.8
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	8	2.8
(2,2909)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	4	2.8
(2,2909)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	9	2.8
(2,2740)	2:112:B:LEU:HD22	1:11:A:TYR:HE1	6	2.8
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	8	2.8
(2,978)	2:127:B:LEU:HD23	2:103:B:TYR:HE2	4	2.8
(2,978)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	9	2.8
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	3	2.79
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	9	2.78
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	2	2.77
(2,2909)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	3	2.77
(2,978)	2:127:B:LEU:HD22	2:103:B:TYR:HE2	3	2.77
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	2	2.74
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	2	2.74
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	2	2.74
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	2.72
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	6	2.7
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	7	2.7
(2,4078)	1:11:A:TYR:HD1	2:109:B:LEU:HA	8	2.7
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	9	2.7
(2,799)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	4	2.7
(2,2909)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	8	2.68
(2,978)	2:127:B:LEU:HD21	2:103:B:TYR:HE2	8	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,759)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	1	2.68
(2,2599)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	1	2.66
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	3	2.64
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	3	2.64
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	5	2.64
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	3	2.64
(2,3423)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	8	2.6
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	1	2.6
(2,1027)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	4	2.6
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	3	2.56
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	1	2.55
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	4	2.55
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	5	2.55
(2,3423)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	6	2.55
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	6	2.55
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	3	2.54
(2,3423)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	5	2.54
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	8	2.53
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	3	2.52
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	9	2.51
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	7	2.51
(2,2975)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	4	2.51
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	2	2.5
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	4	2.5
(2,2656)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	8	2.5
(2,3499)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	5	2.49
(2,3223)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	5	2.49
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	2	2.49
(2,1209)	2:159:B:ILE:HD12	1:11:A:TYR:HE2	5	2.49
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	6	2.46
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	6	2.46
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	2.45
(2,3336)	1:15:A:ILE:HD13	2:109:B:LEU:HD22	4	2.45
(2,2656)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	6	2.45
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	2	2.44
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	9	2.44
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	3	2.44
(2,2656)	2:105:B:ALA:HB3	1:11:A:TYR:HD2	5	2.44
(2,1027)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	10	2.44
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	8	2.43
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	7	2.43
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	4	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2101)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	8	2.43
(2,396)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	8	2.43
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	6	2.42
(2,4427)	1:11:A:TYR:HD1	2:109:B:LEU:HA	7	2.42
(2,2101)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	9	2.42
(2,1027)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	2	2.42
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	4	2.42
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	1	2.41
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	10	2.41
(2,396)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	9	2.41
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	5	2.39
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	5	2.39
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	5	2.39
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	4	2.36
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	3	2.36
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	9	2.36
(2,3435)	1:15:A:ILE:HD13	2:109:B:LEU:HD22	4	2.35
(2,2975)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	10	2.35
(2,2101)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	1	2.35
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	3	2.35
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	1	2.34
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	4	2.34
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	5	2.34
(2,3008)	2:138:B:ARG:HG3	2:103:B:TYR:HD1	10	2.34
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	9	2.34
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	7	2.34
(2,1027)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	3	2.34
(2,396)	1:10:A:ILE:HG21	1:11:A:TYR:HD2	1	2.34
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	7	2.34
(2,2975)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	2	2.33
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	2	2.33
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	7	2.33
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	10	2.33
(2,1027)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	8	2.33
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	10	2.32
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	10	2.32
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	3	2.31
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	10	2.31
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	8	2.31
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	2.31
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	9	2.3
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	1	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	2	2.29
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD23	7	2.29
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	5	2.29
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	2	2.27
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	3	2.27
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	4	2.27
(2,3423)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	4	2.26
(2,3386)	1:37:A:VAL:HG11	2:109:B:LEU:HD12	4	2.26
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	2	2.26
(2,2975)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	3	2.25
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	2.24
(2,2975)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	8	2.24
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	6	2.24
(2,1027)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	1	2.24
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	8	2.23
(2,2101)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	2	2.23
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	8	2.22
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	1	2.22
(2,2623)	1:11:A:TYR:HD2	1:14:A:LEU:HD22	9	2.22
(2,1027)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	5	2.22
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	7	2.22
(2,396)	1:10:A:ILE:HG22	1:11:A:TYR:HD2	2	2.22
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	6	2.21
(2,4573)	1:11:A:TYR:HD1	2:109:B:LEU:HA	7	2.21
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	6	2.21
(2,2656)	2:105:B:ALA:HB1	1:11:A:TYR:HD2	4	2.16
(2,2975)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	1	2.15
(2,2623)	1:11:A:TYR:HD1	2:112:B:LEU:HD23	3	2.15
(2,2975)	2:134:B:ALA:HB3	2:103:B:TYR:HE2	5	2.13
(2,1027)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	6	2.13
(2,1027)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	7	2.12
(2,2975)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	6	2.04
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	9	2.04
(2,2975)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	7	2.03
(2,842)	2:109:B:LEU:HD23	1:12:A:SER:HA	4	2.03
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	5	2.03
(2,2709)	2:109:B:LEU:HD23	1:12:A:SER:HA	4	2.02
(2,3300)	1:2:A:ALA:HB3	2:152:B:GLU:HG3	8	2.0
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	9	2.0
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	4	2.0
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	8	1.99
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	10	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1391)	1:24:A:THR:HG21	1:27:A:LYS:HE3	2	1.99
(2,3500)	2:159:B:ILE:HD11	1:59:A:LEU:HD12	6	1.98
(2,762)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	1	1.98
(2,3500)	2:159:B:ILE:HD11	1:59:A:LEU:HD12	7	1.97
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	8	1.97
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	10	1.97
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	5	1.97
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	8	1.97
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	3	1.96
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	10	1.96
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	10	1.96
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	2	1.95
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	4	1.95
(2,3500)	2:159:B:ILE:HD11	1:59:A:LEU:HD11	2	1.94
(2,3500)	2:159:B:ILE:HD13	1:59:A:LEU:HD12	10	1.94
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	2	1.94
(2,3500)	2:159:B:ILE:HD11	1:59:A:LEU:HD12	3	1.93
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	2	1.93
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	6	1.93
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	7	1.93
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD23	7	1.93
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	5	1.92
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	8	1.92
(2,3500)	2:159:B:ILE:HD13	1:59:A:LEU:HD12	5	1.91
(2,3500)	2:159:B:ILE:HD11	1:59:A:LEU:HD12	8	1.91
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	2	1.91
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	4	1.9
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	5	1.9
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	7	1.9
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	6	1.9
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	7	1.9
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	3	1.9
(2,3269)	2:165:B:VAL:H	2:165:B:VAL:HG21	7	1.89
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	3	1.89
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	7	1.89
(2,1262)	2:155:B:ILE:HG13	1:7:A:LEU:HD21	1	1.89
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	4	1.88
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	6	1.88
(2,1027)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	9	1.88
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	3	1.88
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	4	1.88
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	6	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD22	8	1.88
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	9	1.87
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	2	1.87
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	4	1.86
(2,3300)	1:2:A:ALA:HB3	2:152:B:GLU:HG3	7	1.86
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD21	1	1.86
(2,770)	1:11:A:TYR:HD2	1:14:A:LEU:HD22	9	1.86
(2,3500)	2:159:B:ILE:HD12	1:59:A:LEU:HD12	4	1.85
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	6	1.85
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	10	1.85
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	1	1.84
(2,831)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	1.84
(2,3456)	1:15:A:ILE:HD12	2:126:B:ILE:HD12	4	1.83
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	3	1.82
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	8	1.81
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	1	1.8
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	5	1.8
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	7	1.8
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	3	1.8
(2,2975)	2:134:B:ALA:HB2	2:103:B:TYR:HE2	9	1.79
(2,770)	1:11:A:TYR:HD1	2:112:B:LEU:HD23	3	1.79
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	4	1.78
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	6	1.78
(2,795)	2:104:B:VAL:HG12	2:103:B:TYR:HA	8	1.78
(2,595)	1:37:A:VAL:HG11	1:39:A:VAL:HA	8	1.78
(2,3500)	2:159:B:ILE:HD12	1:59:A:LEU:HD12	9	1.77
(2,2622)	1:11:A:TYR:HD1	1:7:A:LEU:HB3	1	1.77
(2,2583)	1:61:A:CYS:HB3	1:65:A:ALA:HB3	2	1.77
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD23	10	1.77
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	2	1.76
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	10	1.76
(2,1242)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.76
(2,595)	1:37:A:VAL:HG11	1:39:A:VAL:HA	6	1.76
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	1	1.75
(2,3826)	2:120:B:ALA:H	2:121:B:LYS:HB3	9	1.74
(2,3443)	2:110:B:ALA:HB3	1:37:A:VAL:HG12	8	1.74
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	8	1.74
(2,2695)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	1.74
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	10	1.74
(2,3443)	2:110:B:ALA:HB1	1:37:A:VAL:HG12	9	1.73
(2,2583)	1:61:A:CYS:HB3	1:65:A:ALA:HB3	5	1.73
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	10	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	5	1.72
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	3	1.71
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	7	1.7
(2,1266)	1:1:A:MET:HG2	2:152:B:GLU:HG3	9	1.7
(2,1262)	2:155:B:ILE:HG13	1:7:A:LEU:HD23	8	1.7
(2,1182)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	1	1.7
(2,3500)	2:159:B:ILE:HD12	1:59:A:LEU:HD11	1	1.69
(2,2187)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	8	1.69
(2,1243)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.69
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	9	1.68
(2,3274)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.68
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	3	1.68
(2,2245)	1:24:A:THR:HG21	1:27:A:LYS:HE3	2	1.68
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	6	1.68
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	9	1.68
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	10	1.67
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	10	1.66
(2,3443)	2:110:B:ALA:HB3	1:37:A:VAL:HG12	4	1.66
(2,3272)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.66
(2,2598)	1:11:A:TYR:HE1	1:7:A:LEU:HB3	1	1.66
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	1	1.66
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD23	6	1.66
(2,595)	1:37:A:VAL:HG11	1:39:A:VAL:HA	4	1.66
(2,3183)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	1	1.65
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	6	1.65
(2,1948)	2:154:B:VAL:HG23	2:151:B:ILE:HG13	1	1.65
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	4	1.65
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD21	8	1.65
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	5	1.64
(2,3443)	2:110:B:ALA:HB3	1:37:A:VAL:HG12	6	1.64
(2,3195)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	8	1.64
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	2	1.64
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	3	1.64
(2,841)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	4	1.64
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	3	1.64
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG12	8	1.63
(2,1186)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	8	1.63
(2,832)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	1.63
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	8	1.62
(2,1266)	1:1:A:MET:HG3	2:152:B:GLU:HG3	4	1.62
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	2	1.61
(2,3510)	2:162:B:LEU:HD12	1:56:A:ILE:HG13	7	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	10	1.61
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	4	1.61
(2,951)	2:125:B:LYS:HD3	2:129:B:SER:HB3	5	1.61
(2,595)	1:37:A:VAL:HG12	1:39:A:VAL:HA	10	1.61
(2,3443)	2:110:B:ALA:HB3	1:37:A:VAL:HG12	5	1.6
(2,1182)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	5	1.6
(2,792)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	10	1.6
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD11	10	1.6
(2,341)	1:1:A:MET:HG3	1:7:A:LEU:HD21	1	1.6
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	6	1.59
(2,3510)	2:162:B:LEU:HD12	1:56:A:ILE:HG13	10	1.59
(2,3456)	1:15:A:ILE:HD11	2:126:B:ILE:HD12	8	1.59
(2,3443)	2:110:B:ALA:HB1	1:37:A:VAL:HG12	3	1.59
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	2	1.59
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	9	1.59
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD11	1	1.59
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	4	1.58
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	6	1.58
(2,1948)	2:154:B:VAL:HG13	2:155:B:ILE:HG12	10	1.58
(2,1182)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	2	1.58
(2,3443)	2:110:B:ALA:HB1	1:37:A:VAL:HG12	7	1.57
(2,3395)	1:39:A:VAL:HG21	2:109:B:LEU:HD13	1	1.57
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	5	1.57
(2,1182)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	9	1.57
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	6	1.57
(2,595)	1:37:A:VAL:HG12	1:39:A:VAL:HA	2	1.57
(2,331)	2:165:B:VAL:H	2:165:B:VAL:HG21	7	1.57
(2,4011)	1:8:A:ALA:HA	1:11:A:TYR:HD1	7	1.56
(2,3443)	2:110:B:ALA:HB1	1:37:A:VAL:HG13	10	1.56
(2,3410)	1:60:A:ILE:HD13	2:159:B:ILE:HG23	2	1.56
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD23	10	1.56
(2,1520)	1:47:A:PHE:HA	1:46:A:LEU:HD13	6	1.56
(2,595)	1:37:A:VAL:HG11	1:39:A:VAL:HA	9	1.56
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD11	7	1.56
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	1	1.55
(2,3510)	2:162:B:LEU:HD13	1:56:A:ILE:HG13	6	1.55
(2,3443)	2:110:B:ALA:HB1	1:37:A:VAL:HG13	1	1.55
(2,3443)	2:110:B:ALA:HB3	1:37:A:VAL:HG13	2	1.55
(2,3410)	1:60:A:ILE:HD13	2:159:B:ILE:HG23	1	1.55
(2,3410)	1:60:A:ILE:HD12	2:159:B:ILE:HG21	5	1.55
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	5	1.55
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	7	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3510)	2:162:B:LEU:HD11	1:56:A:ILE:HG13	1	1.54
(2,3183)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	5	1.54
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD23	10	1.54
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	7	1.54
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	1	1.54
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	4	1.53
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	5	1.53
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	8	1.53
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	1.53
(2,3486)	2:132:B:ILE:HG21	1:16:A:LEU:HD11	8	1.53
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	4	1.53
(2,3183)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	2	1.53
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	4	1.53
(2,2011)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.53
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	1	1.53
(2,1266)	1:1:A:MET:HG2	2:152:B:GLU:HG3	10	1.53
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	2	1.53
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	9	1.53
(2,1057)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	10	1.53
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	4	1.53
(2,841)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	10	1.53
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD21	7	1.53
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	6	1.52
(2,3183)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	9	1.52
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	9	1.52
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	5	1.52
(2,595)	1:37:A:VAL:HG11	1:39:A:VAL:HA	5	1.52
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	2	1.51
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	9	1.51
(2,1182)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	7	1.51
(2,1060)	2:139:B:LEU:HD23	2:124:B:LYS:HD2	5	1.51
(2,841)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	8	1.51
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	5	1.5
(2,4241)	1:11:A:TYR:HA	1:11:A:TYR:HD2	3	1.5
(2,3437)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	4	1.5
(2,2706)	1:8:A:ALA:HA	2:109:B:LEU:HD12	4	1.5
(2,3410)	1:60:A:ILE:HD13	2:159:B:ILE:HG23	3	1.49
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	5	1.49
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	5	1.49
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	1	1.49
(2,1948)	2:154:B:VAL:HG13	2:155:B:ILE:HG12	2	1.49
(2,595)	1:37:A:VAL:HG11	1:39:A:VAL:HA	7	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3410)	1:60:A:ILE:HD12	2:159:B:ILE:HG21	4	1.48
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	10	1.48
(2,1182)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	6	1.48
(2,513)	1:27:A:LYS:HG3	1:28:A:ILE:HD11	2	1.48
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	8	1.47
(2,2647)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	10	1.47
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	8	1.47
(2,1765)	2:126:B:ILE:HD12	2:125:B:LYS:HD2	4	1.47
(2,1182)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	3	1.47
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	2	1.47
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	9	1.46
(2,3183)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	7	1.46
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	2	1.46
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	9	1.46
(2,1642)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	1.46
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD21	2	1.46
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	2	1.46
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	5	1.45
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	3	1.45
(2,1948)	2:154:B:VAL:HG13	2:155:B:ILE:HG12	4	1.45
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD23	6	1.45
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	5	1.45
(2,841)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	1	1.45
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	1	1.44
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	4	1.44
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	5	1.44
(2,3510)	2:162:B:LEU:HD13	1:56:A:ILE:HG13	4	1.44
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG12	7	1.44
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	1	1.44
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD21	8	1.44
(2,1182)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	10	1.44
(2,3183)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	6	1.43
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	6	1.43
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD23	6	1.43
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	6	1.43
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	4	1.43
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG12	7	1.43
(2,1182)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	4	1.43
(2,1182)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	8	1.43
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	1	1.42
(2,3410)	1:60:A:ILE:HD13	2:159:B:ILE:HG23	9	1.42
(2,3395)	1:39:A:VAL:HG21	2:109:B:LEU:HD13	3	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3395)	1:39:A:VAL:HG21	2:109:B:LEU:HD12	6	1.42
(2,3183)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	3	1.42
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD21	8	1.42
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	2	1.42
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	7	1.42
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	3	1.42
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	3	1.41
(2,3513)	2:155:B:ILE:HG23	1:11:A:TYR:HE2	5	1.41
(2,2694)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	1.41
(2,2626)	2:101:B:MET:HE1	2:102:B:ARG:H	1	1.41
(2,2626)	2:101:B:MET:HE2	2:103:B:TYR:H	3	1.41
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	3	1.41
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	9	1.41
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	2	1.4
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	6	1.4
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	9	1.4
(2,3510)	2:162:B:LEU:HD12	1:56:A:ILE:HG13	3	1.4
(2,3509)	2:159:B:ILE:HG21	1:10:A:ILE:HG12	4	1.4
(2,3437)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	10	1.4
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	8	1.4
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	10	1.4
(2,2703)	2:109:B:LEU:HD21	2:109:B:LEU:H	4	1.4
(2,2626)	2:101:B:MET:HE3	2:104:B:VAL:H	7	1.4
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	6	1.4
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	2	1.4
(2,1645)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	1.4
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	2	1.4
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	4	1.4
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	2	1.39
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	1	1.39
(2,3183)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	10	1.39
(2,1948)	2:154:B:VAL:HG23	2:149:B:LYS:HD3	3	1.39
(2,1714)	2:121:B:LYS:HD2	2:121:B:LYS:HB3	1	1.39
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	4	1.39
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	10	1.39
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB3	3	1.39
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD21	5	1.39
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	9	1.38
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	7	1.38
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	5	1.38
(2,3322)	1:10:A:ILE:HD11	2:159:B:ILE:HG22	1	1.38
(2,3183)	2:155:B:ILE:HG22	2:159:B:ILE:HG12	4	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3183)	2:155:B:ILE:HG23	2:159:B:ILE:HG12	8	1.38
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	4	1.38
(2,2022)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.38
(2,1948)	2:154:B:VAL:HG12	2:155:B:ILE:HG12	9	1.38
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	3	1.38
(2,1714)	2:121:B:LYS:HD2	2:121:B:LYS:HB3	5	1.38
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	8	1.38
(2,1625)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	10	1.38
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG21	6	1.38
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	3	1.38
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	9	1.37
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	9	1.37
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	4	1.37
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	5	1.37
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	1.37
(2,3437)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	8	1.37
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	2	1.37
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG21	4	1.37
(2,2645)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	10	1.37
(2,1714)	2:121:B:LYS:HD3	2:121:B:LYS:HB3	7	1.37
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	1	1.37
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	6	1.36
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	8	1.36
(2,3486)	2:132:B:ILE:HG23	1:16:A:LEU:HD11	7	1.36
(2,3395)	1:39:A:VAL:HG23	2:112:B:LEU:HD22	7	1.36
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	9	1.36
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD21	6	1.36
(2,1948)	2:154:B:VAL:HG23	2:151:B:ILE:HG13	5	1.36
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG21	1	1.36
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	6	1.36
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	7	1.36
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	2	1.35
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	9	1.35
(2,3486)	2:132:B:ILE:HG21	1:16:A:LEU:HD13	5	1.35
(2,3191)	2:156:B:ALA:HB3	2:153:B:ASP:HB2	6	1.35
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG12	7	1.35
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	10	1.35
(2,792)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	8	1.35
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD11	6	1.35
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	10	1.34
(2,4013)	1:11:A:TYR:HA	1:11:A:TYR:HD2	3	1.34
(2,3486)	2:132:B:ILE:HG23	1:16:A:LEU:HD13	9	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2318)	1:32:A:ILE:HD12	1:9:A:CYS:H	3	1.34
(2,2188)	1:18:A:ASP:HB2	1:19:A:ASP:HB2	8	1.34
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG12	4	1.34
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD11	5	1.34
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG21	7	1.34
(2,1063)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	6	1.34
(2,841)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	3	1.34
(2,836)	1:8:A:ALA:HA	2:109:B:LEU:HD12	4	1.34
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	9	1.34
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	7	1.34
(2,3510)	2:162:B:LEU:HD12	1:56:A:ILE:HG13	9	1.33
(2,3322)	1:10:A:ILE:HD11	2:159:B:ILE:HG22	3	1.33
(2,3281)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.33
(2,2583)	1:61:A:CYS:HB2	1:65:A:ALA:HB1	7	1.33
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	2	1.33
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	7	1.33
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	4	1.33
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	8	1.32
(2,3486)	2:132:B:ILE:HG22	1:16:A:LEU:HD12	3	1.32
(2,3315)	1:8:A:ALA:HB2	2:109:B:LEU:HD12	4	1.32
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD21	7	1.32
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	9	1.32
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	2	1.32
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	8	1.32
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	6	1.31
(2,4411)	1:11:A:TYR:HD1	2:109:B:LEU:HA	7	1.31
(2,3437)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	1	1.31
(2,2852)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	7	1.31
(2,1948)	2:154:B:VAL:HG12	2:155:B:ILE:HG12	7	1.31
(2,1765)	2:126:B:ILE:HD12	2:125:B:LYS:HD2	8	1.31
(2,1714)	2:121:B:LYS:HD2	2:121:B:LYS:HB3	6	1.31
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	4	1.31
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	5	1.31
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	6	1.31
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	9	1.31
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.31
(2,940)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	7	1.31
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	5	1.31
(2,186)	2:111:B:ALA:H	2:109:B:LEU:HD11	2	1.31
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	4	1.3
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	7	1.3
(2,3486)	2:132:B:ILE:HG22	1:16:A:LEU:HD11	10	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB3	3	1.3
(2,3023)	2:139:B:LEU:HD22	2:103:B:TYR:HD1	10	1.3
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD21	7	1.3
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	7	1.3
(2,1063)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	2	1.3
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	1	1.29
(2,3177)	2:154:B:VAL:HG12	2:146:B:LEU:HD11	6	1.29
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	3	1.29
(2,1208)	2:159:B:ILE:HA	2:159:B:ILE:HD13	3	1.29
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	4	1.29
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	8	1.29
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	10	1.29
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG13	4	1.29
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	10	1.28
(2,3428)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	5	1.28
(2,3427)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	5	1.28
(2,3267)	2:165:B:VAL:HA	2:165:B:VAL:HG12	7	1.28
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	7	1.28
(2,3099)	2:146:B:LEU:HD23	2:149:B:LYS:HE3	8	1.28
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	4	1.28
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	1.28
(2,3177)	2:154:B:VAL:HG12	2:146:B:LEU:HD11	8	1.27
(2,2852)	2:123:B:ILE:HG21	2:103:B:TYR:HE2	2	1.27
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	6	1.27
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	10	1.27
(2,940)	2:123:B:ILE:HG21	2:103:B:TYR:HE2	2	1.27
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	5	1.26
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	5	1.26
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	4	1.26
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	4	1.26
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	2	1.26
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	1	1.26
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG13	9	1.26
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	4	1.25
(2,2852)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	3	1.25
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD21	2	1.25
(2,1238)	2:165:B:VAL:HA	2:165:B:VAL:HG12	7	1.25
(2,940)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	3	1.25
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	8	1.24
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	10	1.24
(2,3510)	2:162:B:LEU:HD11	1:56:A:ILE:HG13	5	1.24
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	2	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	8	1.24
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	5	1.24
(2,2626)	2:101:B:MET:HE2	2:102:B:ARG:H	8	1.24
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	3	1.24
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	10	1.24
(2,2318)	1:32:A:ILE:HD12	1:9:A:CYS:H	9	1.24
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	8	1.24
(2,1643)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	1.24
(2,1063)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	7	1.24
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	4	1.24
(2,369)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	1.24
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG13	7	1.24
(2,3513)	2:155:B:ILE:HG21	1:11:A:TYR:HE2	6	1.23
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	4	1.23
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	5	1.23
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	6	1.23
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	9	1.23
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.23
(2,3074)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	4	1.23
(2,2852)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	10	1.23
(2,2647)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	8	1.23
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD21	2	1.23
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	7	1.23
(2,2013)	2:165:B:VAL:HA	2:165:B:VAL:HG12	7	1.23
(2,1105)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	4	1.23
(2,940)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	10	1.23
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	5	1.22
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	1	1.22
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	7	1.22
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	6	1.22
(2,2852)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	4	1.22
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	7	1.22
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	5	1.22
(2,2368)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	3	1.22
(2,2318)	1:32:A:ILE:HD12	1:9:A:CYS:H	5	1.22
(2,1063)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	3	1.22
(2,940)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	4	1.22
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	8	1.22
(2,790)	2:104:B:VAL:HG21	2:146:B:LEU:HD23	10	1.22
(2,374)	1:8:A:ALA:HA	2:109:B:LEU:HD12	4	1.22
(2,4572)	1:11:A:TYR:HE1	2:108:B:LEU:HA	3	1.21
(2,3502)	2:159:B:ILE:HD12	1:60:A:ILE:HG13	8	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3486)	2:132:B:ILE:HG23	1:16:A:LEU:HD13	2	1.21
(2,3224)	2:159:B:ILE:HA	2:159:B:ILE:HD13	3	1.21
(2,3205)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	8	1.21
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD23	10	1.21
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	7	1.21
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	7	1.21
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	8	1.21
(2,1063)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	8	1.21
(2,841)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	5	1.21
(2,186)	2:111:B:ALA:H	2:109:B:LEU:HD11	6	1.21
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	2	1.2
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	4	1.2
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	10	1.2
(2,3437)	2:109:B:LEU:HD11	1:11:A:TYR:HD1	3	1.2
(2,3428)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	6	1.2
(2,3427)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	6	1.2
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	2	1.2
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	4	1.2
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	5	1.2
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	6	1.2
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	9	1.2
(2,596)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	3	1.2
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD13	8	1.2
(2,369)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	1	1.2
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	1	1.19
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	8	1.19
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	10	1.19
(2,2729)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	9	1.19
(2,2181)	1:17:A:HIS:HB3	1:56:A:ILE:HG23	5	1.19
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.19
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD21	9	1.19
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG13	5	1.19
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	3	1.18
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	6	1.18
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	8	1.18
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	3	1.18
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	5	1.18
(2,3513)	2:155:B:ILE:HG21	1:11:A:TYR:HE2	7	1.18
(2,3486)	2:132:B:ILE:HG22	1:16:A:LEU:HD12	1	1.18
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	1.18
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	4	1.18
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	4	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD21	5	1.18
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	7	1.18
(2,827)	2:108:B:LEU:HD22	2:104:B:VAL:HB	3	1.18
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	3	1.17
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	3	1.17
(2,3428)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	8	1.17
(2,3427)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	8	1.17
(2,2729)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	3	1.17
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG23	5	1.17
(2,2256)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	2	1.17
(2,1200)	2:159:B:ILE:HA	2:159:B:ILE:HD13	3	1.17
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	4	1.17
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD12	1	1.17
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	2	1.16
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	4	1.16
(2,3428)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	7	1.16
(2,3427)	2:108:B:LEU:HD22	1:15:A:ILE:HD13	7	1.16
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB3	4	1.16
(2,2976)	2:134:B:ALA:HB2	2:135:B:ASP:HB3	8	1.16
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD21	5	1.16
(2,1843)	2:139:B:LEU:HD13	2:143:B:ILE:HD11	6	1.16
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	1	1.16
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	6	1.15
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	1	1.15
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	3	1.15
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	6	1.15
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	6	1.15
(2,3513)	2:155:B:ILE:HG21	1:11:A:TYR:HE2	2	1.15
(2,3486)	2:132:B:ILE:HG22	1:16:A:LEU:HD13	4	1.15
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	2	1.15
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	9	1.15
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB2	10	1.15
(2,2729)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	4	1.15
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	1.15
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	8	1.15
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	3	1.15
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	7	1.15
(2,841)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	2	1.15
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	1.15
(2,752)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	1	1.15
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD13	9	1.15
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	7	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	9	1.14
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	8	1.14
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	7	1.14
(2,3513)	2:155:B:ILE:HG23	1:11:A:TYR:HE2	9	1.14
(2,3173)	2:154:B:VAL:HG23	2:151:B:ILE:HG12	1	1.14
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	1	1.14
(2,2626)	2:101:B:MET:HE1	2:102:B:ARG:H	9	1.14
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	8	1.14
(2,1994)	2:161:B:LYS:HE2	2:161:B:LYS:HB3	3	1.14
(2,1625)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	8	1.14
(2,841)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	6	1.14
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	7	1.14
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD13	4	1.14
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	1	1.13
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	10	1.13
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	1	1.13
(2,3513)	2:155:B:ILE:HG23	1:11:A:TYR:HE2	4	1.13
(2,3513)	2:155:B:ILE:HG21	1:11:A:TYR:HE2	8	1.13
(2,3428)	2:108:B:LEU:HD21	1:15:A:ILE:HD13	3	1.13
(2,3428)	2:108:B:LEU:HD22	1:15:A:ILE:HD11	4	1.13
(2,3427)	2:108:B:LEU:HD21	1:15:A:ILE:HD13	3	1.13
(2,3427)	2:108:B:LEU:HD22	1:15:A:ILE:HD11	4	1.13
(2,3177)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	7	1.13
(2,3101)	2:146:B:LEU:H	2:146:B:LEU:HD22	1	1.13
(2,2976)	2:134:B:ALA:HB2	2:135:B:ASP:HB3	3	1.13
(2,2742)	2:112:B:LEU:HD22	2:109:B:LEU:HD12	10	1.13
(2,2645)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	8	1.13
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	3	1.13
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	9	1.13
(2,2256)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	5	1.13
(2,2181)	1:17:A:HIS:HB3	1:56:A:ILE:HG23	10	1.13
(2,1874)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	4	1.13
(2,1266)	1:1:A:MET:HG3	2:152:B:GLU:HG3	8	1.13
(2,1173)	2:154:B:VAL:HG12	2:146:B:LEU:HD11	6	1.13
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	4	1.13
(2,841)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	7	1.13
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD23	4	1.13
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD13	9	1.13
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG11	10	1.13
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD13	6	1.13
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD11	8	1.13
(2,3513)	2:155:B:ILE:HG23	1:11:A:TYR:HE2	3	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	10	1.12
(2,2976)	2:134:B:ALA:HB3	2:135:B:ASP:HB2	7	1.12
(2,1486)	1:39:A:VAL:HG22	1:5:A:SER:HA	3	1.12
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	2	1.12
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	9	1.12
(2,855)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	9	1.12
(2,841)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	9	1.12
(2,181)	2:107:B:TYR:H	2:146:B:LEU:HD11	4	1.12
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD13	2	1.12
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	5	1.11
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	9	1.11
(2,3454)	1:35:A:ALA:HB2	2:126:B:ILE:HD12	2	1.11
(2,3387)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	3	1.11
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	1	1.11
(2,2861)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	6	1.11
(2,2729)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	2	1.11
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	3	1.11
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	1	1.11
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	4	1.11
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	6	1.11
(2,1486)	1:39:A:VAL:HG13	1:5:A:SER:HA	1	1.11
(2,1173)	2:154:B:VAL:HG12	2:146:B:LEU:HD11	8	1.11
(2,951)	2:125:B:LYS:HD3	2:129:B:SER:HB3	10	1.11
(2,855)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	3	1.11
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	1.11
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD11	7	1.11
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	4	1.1
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	8	1.1
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	4	1.1
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	8	1.1
(2,3513)	2:155:B:ILE:HG23	1:11:A:TYR:HE2	10	1.1
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG12	9	1.1
(2,3428)	2:108:B:LEU:HD22	1:7:A:LEU:HD22	10	1.1
(2,3427)	2:108:B:LEU:HD22	1:7:A:LEU:HD22	10	1.1
(2,2852)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	5	1.1
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD23	6	1.1
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	5	1.1
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	10	1.1
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	8	1.1
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	3	1.1
(2,1994)	2:161:B:LYS:HE3	2:161:B:LYS:HB2	8	1.1
(2,940)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	5	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	8	1.1
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	3	1.1
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG13	8	1.1
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	2	1.09
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	1	1.09
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	8	1.09
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	2	1.09
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	4	1.09
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	8	1.09
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD21	8	1.09
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	8	1.09
(2,1843)	2:139:B:LEU:HD12	2:143:B:ILE:HD11	7	1.09
(2,1764)	2:126:B:ILE:HD13	2:109:B:LEU:HD22	4	1.09
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	1	1.09
(2,855)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	4	1.09
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	2	1.09
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	7	1.09
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD13	5	1.09
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	5	1.08
(2,3488)	2:152:B:GLU:HB2	1:4:A:VAL:HG23	1	1.08
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	6	1.08
(2,3437)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	5	1.08
(2,3203)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	8	1.08
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	7	1.08
(2,2569)	1:60:A:ILE:H	1:60:A:ILE:HD11	2	1.08
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	1	1.08
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	1	1.08
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	4	1.08
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	10	1.08
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	5	1.08
(2,1486)	1:39:A:VAL:HG12	1:5:A:SER:HA	5	1.08
(2,1486)	1:39:A:VAL:HG22	1:5:A:SER:HA	9	1.08
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	8	1.08
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	6	1.07
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	2	1.07
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB3	7	1.07
(2,2852)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	6	1.07
(2,2852)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	9	1.07
(2,2368)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	1	1.07
(2,2023)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	1.07
(2,1994)	2:161:B:LYS:HE3	2:161:B:LYS:HB2	2	1.07
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	10	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,940)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	6	1.07
(2,940)	2:123:B:ILE:HG22	2:103:B:TYR:HE2	9	1.07
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	4	1.06
(2,3486)	2:132:B:ILE:HG21	1:16:A:LEU:HD13	6	1.06
(2,3300)	1:2:A:ALA:HB1	2:152:B:GLU:HG3	9	1.06
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	8	1.06
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	8	1.06
(2,2729)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	10	1.06
(2,2626)	2:101:B:MET:HE1	2:102:B:ARG:H	4	1.06
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG2	1	1.06
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	2	1.06
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	9	1.06
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	10	1.06
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	10	1.06
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	10	1.06
(2,1393)	1:24:A:THR:HG22	1:26:A:ASP:HB2	3	1.06
(2,596)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	1	1.06
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	9	1.06
(2,181)	2:107:B:TYR:H	2:146:B:LEU:HD13	3	1.06
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	3	1.06
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	9	1.06
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD12	3	1.06
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	9	1.05
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	6	1.05
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	2	1.05
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	4	1.05
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	5	1.05
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	6	1.05
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	9	1.05
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	4	1.05
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	1	1.05
(2,2729)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	8	1.05
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	5	1.05
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	1	1.05
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	2	1.05
(2,2181)	1:17:A:HIS:HB3	1:56:A:ILE:HG23	7	1.05
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	4	1.05
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD12	7	1.05
(2,1486)	1:39:A:VAL:HG11	1:5:A:SER:HA	8	1.05
(2,1262)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	10	1.05
(2,855)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	2	1.05
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	3	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	5	1.05
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	1.04
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	4	1.04
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	7	1.04
(2,2076)	1:8:A:ALA:HA	2:109:B:LEU:HD12	4	1.04
(2,1996)	2:162:B:LEU:HA	2:165:B:VAL:HG22	3	1.04
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG2	7	1.04
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	6	1.04
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	1	1.04
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG11	1	1.04
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	6	1.04
(2,46)	1:17:A:HIS:H	1:16:A:LEU:HD11	10	1.04
(2,4230)	1:8:A:ALA:HA	1:11:A:TYR:HD1	7	1.03
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	8	1.03
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	7	1.03
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	5	1.03
(2,2976)	2:134:B:ALA:HB2	2:135:B:ASP:HB3	9	1.03
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	7	1.03
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	1.03
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	9	1.03
(2,2181)	1:17:A:HIS:HB3	1:56:A:ILE:HG23	2	1.03
(2,1843)	2:139:B:LEU:HD13	2:143:B:ILE:HD12	2	1.03
(2,1843)	2:139:B:LEU:HD11	2:143:B:ILE:HD13	8	1.03
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	2	1.03
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	2	1.03
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	2	1.03
(2,1746)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	6	1.03
(2,1266)	1:1:A:MET:HG3	2:152:B:GLU:HG3	5	1.03
(2,950)	2:125:B:LYS:HB2	2:122:B:ASP:HB3	5	1.03
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	6	1.03
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	7	1.03
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD3	6	1.03
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	4	1.03
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	9	1.03
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	1	1.03
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	4	1.03
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	10	1.03
(2,3300)	1:2:A:ALA:HB1	2:152:B:GLU:HG3	2	1.02
(2,3213)	2:159:B:ILE:HA	2:159:B:ILE:HD13	3	1.02
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	10	1.02
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB3	5	1.02
(2,2729)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	5	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2729)	2:111:B:ALA:HB2	2:151:B:ILE:HD12	7	1.02
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	10	1.02
(2,1486)	1:39:A:VAL:HG11	1:5:A:SER:HA	2	1.02
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	1	1.02
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	5	1.02
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	5	1.02
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	2	1.01
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	5	1.01
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	1	1.01
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	8	1.01
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	1	1.01
(2,3515)	2:155:B:ILE:HG13	1:7:A:LEU:HD21	1	1.01
(2,3502)	2:159:B:ILE:HD12	1:60:A:ILE:HG13	3	1.01
(2,3437)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	2	1.01
(2,3351)	1:16:A:LEU:HD12	2:130:B:VAL:HA	10	1.01
(2,3300)	1:2:A:ALA:HB3	2:152:B:GLU:HG3	5	1.01
(2,3173)	2:154:B:VAL:HG21	2:151:B:ILE:HG12	4	1.01
(2,3017)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	1.01
(2,2580)	1:61:A:CYS:HB3	1:60:A:ILE:HG22	1	1.01
(2,1540)	1:56:A:ILE:HA	1:51:A:LEU:HD23	7	1.01
(2,1486)	1:39:A:VAL:HG22	1:5:A:SER:HA	10	1.01
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	4	1.01
(2,152)	1:60:A:ILE:H	1:60:A:ILE:HD11	2	1.01
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	10	1.0
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	10	1.0
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	10	1.0
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	10	1.0
(2,3437)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	6	1.0
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	1.0
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	2	1.0
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	9	1.0
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	4	1.0
(2,1486)	1:39:A:VAL:HG22	1:5:A:SER:HA	4	1.0
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	1	1.0
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	5	1.0
(2,880)	2:116:B:SER:HA	2:151:B:ILE:HD12	10	1.0
(2,855)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	10	1.0
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	6	1.0
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	2	1.0
(2,385)	1:10:A:ILE:HB	1:10:A:ILE:HD11	3	1.0
(2,369)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	6	1.0
(2,186)	2:111:B:ALA:H	1:37:A:VAL:HG13	3	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	9	0.99
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	10	0.99
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	2	0.99
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	3	0.99
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	9	0.99
(2,3437)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	7	0.99
(2,3437)	2:109:B:LEU:HD13	1:11:A:TYR:HD1	9	0.99
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	4	0.99
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	4	0.99
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	4	0.99
(2,855)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	8	0.99
(2,595)	1:37:A:VAL:HG12	2:114:B:GLY:HA3	3	0.99
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD11	5	0.99
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE2	4	0.99
(2,385)	1:10:A:ILE:HB	1:10:A:ILE:HD11	1	0.99
(2,385)	1:10:A:ILE:HB	1:10:A:ILE:HD11	8	0.99
(2,181)	2:107:B:TYR:H	2:146:B:LEU:HD13	1	0.99
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG22	4	0.99
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	1	0.98
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	4	0.98
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	5	0.98
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	2	0.98
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	6	0.98
(2,3502)	2:159:B:ILE:HD12	1:60:A:ILE:HG13	7	0.98
(2,3351)	1:16:A:LEU:HD11	2:130:B:VAL:HA	2	0.98
(2,1929)	2:152:B:GLU:HA	2:155:B:ILE:HD12	9	0.98
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	4	0.98
(2,1809)	2:132:B:ILE:HG22	1:18:A:ASP:HB2	5	0.98
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD21	9	0.98
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	8	0.98
(2,1060)	2:139:B:LEU:HD22	2:124:B:LYS:HD2	8	0.98
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD11	4	0.98
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE2	9	0.98
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	2	0.98
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	8	0.98
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	1	0.97
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	7	0.97
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	4	0.97
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	7	0.97
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	5	0.97
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	7	0.97
(2,3502)	2:159:B:ILE:HD11	1:60:A:ILE:HG13	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3351)	1:16:A:LEU:HD13	2:130:B:VAL:HA	1	0.97
(2,3351)	1:16:A:LEU:HD11	2:130:B:VAL:HA	5	0.97
(2,3300)	1:2:A:ALA:HB3	2:152:B:GLU:HG3	4	0.97
(2,3177)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	10	0.97
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	8	0.97
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD21	7	0.97
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	0.97
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	4	0.97
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	6	0.97
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	9	0.97
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	3	0.97
(2,1173)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	7	0.97
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD13	10	0.97
(2,826)	2:108:B:LEU:HD22	2:104:B:VAL:HB	3	0.97
(2,790)	2:104:B:VAL:HG11	2:146:B:LEU:HD21	8	0.97
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	0.97
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	3	0.97
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	9	0.97
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	1	0.97
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE1	3	0.97
(2,385)	1:10:A:ILE:HB	1:10:A:ILE:HD11	6	0.97
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	8	0.96
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	10	0.96
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	4	0.96
(2,3502)	2:159:B:ILE:HD12	1:60:A:ILE:HG13	6	0.96
(2,3428)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	1	0.96
(2,3427)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	1	0.96
(2,3387)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	1	0.96
(2,3177)	2:154:B:VAL:HG11	2:146:B:LEU:HD21	2	0.96
(2,3175)	2:154:B:VAL:H	2:154:B:VAL:HG23	4	0.96
(2,3175)	2:154:B:VAL:H	2:154:B:VAL:HG23	10	0.96
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD21	9	0.96
(2,2069)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	0.96
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	5	0.96
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	5	0.96
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	5	0.96
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.96
(2,1198)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	8	0.96
(2,1059)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	0.96
(2,855)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	5	0.96
(2,855)	2:111:B:ALA:HB2	2:151:B:ILE:HD12	7	0.96
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	4	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	7	0.95
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	2	0.95
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	2	0.95
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	4	0.95
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	1	0.95
(2,3502)	2:159:B:ILE:HD11	1:60:A:ILE:HG13	9	0.95
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	1	0.95
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	7	0.95
(2,2257)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	2	0.95
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	8	0.95
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG2	4	0.95
(2,1843)	2:139:B:LEU:HD12	2:143:B:ILE:HD13	5	0.95
(2,1486)	1:39:A:VAL:HG22	1:5:A:SER:HA	6	0.95
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	10	0.95
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD23	1	0.95
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	4	0.95
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE2	5	0.95
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	10	0.95
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG12	1	0.95
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	4	0.94
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	3	0.94
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	5	0.94
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	6	0.94
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	10	0.94
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	1	0.94
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	6	0.94
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	7	0.94
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	8	0.94
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	4	0.94
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	2	0.94
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	9	0.94
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB2	3	0.94
(2,2852)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	1	0.94
(2,2852)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	8	0.94
(2,2627)	2:101:B:MET:HE1	2:102:B:ARG:H	1	0.94
(2,2627)	2:101:B:MET:HE2	2:103:B:TYR:H	3	0.94
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	5	0.94
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	9	0.94
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	5	0.94
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	6	0.94
(2,1948)	2:154:B:VAL:HG22	2:149:B:LYS:HD2	6	0.94
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	3	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	3	0.94
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	3	0.94
(2,1658)	2:111:B:ALA:HB2	2:151:B:ILE:HG13	8	0.94
(2,1194)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	8	0.94
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	4	0.94
(2,940)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	1	0.94
(2,940)	2:123:B:ILE:HG23	2:103:B:TYR:HE2	8	0.94
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.94
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	9	0.94
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE2	10	0.94
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	4	0.93
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	9	0.93
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	3	0.93
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	8	0.93
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	6	0.93
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	4	0.93
(2,3502)	2:159:B:ILE:HD11	1:60:A:ILE:HG13	2	0.93
(2,3351)	1:16:A:LEU:HD13	2:130:B:VAL:HA	3	0.93
(2,3173)	2:154:B:VAL:HG21	2:151:B:ILE:HG12	10	0.93
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	6	0.93
(2,2729)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	1	0.93
(2,2729)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	6	0.93
(2,2579)	1:61:A:CYS:HB3	1:62:A:ASN:HD21	9	0.93
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	2	0.93
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	2	0.93
(2,2096)	1:10:A:ILE:HB	1:10:A:ILE:HD11	3	0.93
(2,1824)	2:134:B:ALA:HB3	2:124:B:LYS:HE2	6	0.93
(2,1486)	1:39:A:VAL:HG13	1:5:A:SER:HA	7	0.93
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	2	0.93
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB1	2	0.93
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG22	10	0.93
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG12	3	0.92
(2,3351)	1:16:A:LEU:HD11	2:130:B:VAL:HA	6	0.92
(2,3175)	2:154:B:VAL:H	2:154:B:VAL:HG23	2	0.92
(2,3151)	2:152:B:GLU:HB2	2:151:B:ILE:HG22	3	0.92
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	9	0.92
(2,3113)	2:146:B:LEU:H	2:146:B:LEU:HD22	1	0.92
(2,2945)	2:132:B:ILE:HD12	2:133:B:GLU:H	9	0.92
(2,2627)	2:101:B:MET:HE3	2:104:B:VAL:H	7	0.92
(2,2166)	1:16:A:LEU:HD11	1:27:A:LYS:HE3	2	0.92
(2,2096)	1:10:A:ILE:HB	1:10:A:ILE:HD11	1	0.92
(2,2096)	1:10:A:ILE:HB	1:10:A:ILE:HD11	8	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2069)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	1	0.92
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	4	0.92
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	1	0.92
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	2	0.92
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	3	0.92
(2,370)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	0.92
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	7	0.92
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG22	3	0.92
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	7	0.91
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	8	0.91
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE1	4	0.91
(2,3177)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	5	0.91
(2,3177)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	9	0.91
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	6	0.91
(2,2683)	2:108:B:LEU:HD22	2:104:B:VAL:HB	3	0.91
(2,2257)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	5	0.91
(2,2096)	1:10:A:ILE:HB	1:10:A:ILE:HD11	6	0.91
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD23	4	0.91
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	6	0.91
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	7	0.91
(2,314)	2:153:B:ASP:H	2:151:B:ILE:HG22	3	0.91
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	1	0.91
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG13	3	0.91
(2,4486)	2:133:B:GLU:H	2:133:B:GLU:HB3	2	0.9
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	7	0.9
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	7	0.9
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	5	0.9
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	9	0.9
(2,3351)	1:16:A:LEU:HD11	2:130:B:VAL:HA	4	0.9
(2,3351)	1:16:A:LEU:HD12	2:130:B:VAL:HA	7	0.9
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	2	0.9
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	10	0.9
(2,3173)	2:154:B:VAL:HG23	2:151:B:ILE:HG12	5	0.9
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	7	0.9
(2,2916)	2:128:B:ASP:HB2	2:124:B:LYS:HB3	5	0.9
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD21	2	0.9
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	6	0.9
(2,2267)	1:26:A:ASP:HB2	1:30:A:ALA:HB1	9	0.9
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	1	0.9
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	3	0.9
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG2	10	0.9
(2,1878)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	4	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	6	0.9
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	6	0.9
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD11	6	0.9
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	3	0.9
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	7	0.9
(2,619)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	8	0.9
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	9	0.9
(2,502)	1:26:A:ASP:HB2	1:30:A:ALA:HB1	9	0.9
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	5	0.9
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	9	0.89
(2,4499)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	10	0.89
(2,4097)	2:138:B:ARG:HG3	2:103:B:TYR:HE1	10	0.89
(2,3510)	2:162:B:LEU:HD13	1:56:A:ILE:HG13	8	0.89
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG13	2	0.89
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	6	0.89
(2,3393)	1:37:A:VAL:HG12	2:109:B:LEU:HD13	10	0.89
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	7	0.89
(2,3173)	2:154:B:VAL:HG23	2:151:B:ILE:HG12	6	0.89
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	4	0.89
(2,3099)	2:146:B:LEU:HD23	2:149:B:LYS:HE3	7	0.89
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD23	4	0.89
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	3	0.89
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	9	0.89
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	5	0.89
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	3	0.89
(2,1849)	2:139:B:LEU:HD23	2:124:B:LYS:HD2	5	0.89
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.89
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	8	0.89
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	6	0.89
(2,682)	1:50:A:ALA:HB1	1:46:A:LEU:HB3	1	0.89
(2,595)	1:37:A:VAL:HG13	2:114:B:GLY:HA3	1	0.89
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG22	8	0.89
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	5	0.88
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	6	0.88
(2,3510)	2:162:B:LEU:HD11	1:56:A:ILE:HG13	2	0.88
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	6	0.88
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	7	0.88
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	1	0.88
(2,3351)	1:16:A:LEU:HD12	2:130:B:VAL:HA	8	0.88
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE1	9	0.88
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	1	0.88
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	10	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	3	0.88
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	7	0.88
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	2	0.88
(2,1654)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.88
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG22	4	0.88
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	1	0.88
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	7	0.88
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	10	0.88
(2,370)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	1	0.88
(2,314)	2:153:B:ASP:H	2:151:B:ILE:HG22	4	0.88
(2,219)	2:117:B:SER:H	2:151:B:ILE:HD12	6	0.88
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	1	0.87
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	3	0.87
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	5	0.87
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	7	0.87
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.87
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	10	0.87
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	2	0.87
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	7	0.87
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	8	0.87
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	9	0.87
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	10	0.87
(2,3739)	1:59:A:LEU:H	1:58:A:SER:HB3	3	0.87
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	1	0.87
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG12	5	0.87
(2,3388)	1:37:A:VAL:HG12	2:109:B:LEU:HD13	10	0.87
(2,3370)	1:34:A:ALA:HB3	2:125:B:LYS:HG3	7	0.87
(2,3369)	1:34:A:ALA:HB3	2:125:B:LYS:HG3	7	0.87
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	3	0.87
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	7	0.87
(2,3175)	2:154:B:VAL:H	2:154:B:VAL:HG23	9	0.87
(2,3173)	2:154:B:VAL:HG23	2:151:B:ILE:HG12	7	0.87
(2,2771)	2:116:B:SER:HA	2:151:B:ILE:HD12	5	0.87
(2,2721)	2:110:B:ALA:HB1	2:119:B:SER:H	8	0.87
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	8	0.87
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	5	0.87
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	7	0.87
(2,1809)	2:132:B:ILE:HG22	1:18:A:ASP:HB2	8	0.87
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG22	9	0.87
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	5	0.87
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	4	0.87
(2,838)	2:109:B:LEU:HD22	2:126:B:ILE:HB	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,314)	2:153:B:ASP:H	2:151:B:ILE:HG22	10	0.87
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	3	0.86
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	1	0.86
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	2	0.86
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	4	0.86
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	6	0.86
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	8	0.86
(2,4372)	1:59:A:LEU:HB3	1:59:A:LEU:HG	9	0.86
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	9	0.86
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	2	0.86
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	3	0.86
(2,3502)	2:159:B:ILE:HD11	1:60:A:ILE:HG13	4	0.86
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	9	0.86
(2,3464)	2:129:B:SER:HA	1:30:A:ALA:HA	4	0.86
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	2	0.86
(2,3390)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	3	0.86
(2,3151)	2:152:B:GLU:HB2	2:151:B:ILE:HG22	7	0.86
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	3	0.86
(2,3099)	2:146:B:LEU:HD23	2:149:B:LYS:HE3	5	0.86
(2,2721)	2:110:B:ALA:HB1	2:119:B:SER:H	5	0.86
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	0.86
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	6	0.86
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG13	3	0.86
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.86
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	9	0.86
(2,1843)	2:139:B:LEU:HD12	2:143:B:ILE:HD11	9	0.86
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	2	0.86
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	10	0.86
(2,950)	2:125:B:LYS:HB2	2:122:B:ASP:HB3	10	0.86
(2,855)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	1	0.86
(2,855)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	6	0.86
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	6	0.86
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG22	4	0.86
(2,513)	1:27:A:LYS:HG2	1:28:A:ILE:HD13	3	0.86
(2,4521)	2:145:B:GLU:HG2	2:145:B:GLU:H	8	0.85
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	6	0.85
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	6	0.85
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	3	0.85
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	4	0.85
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	5	0.85
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	4	0.85
(2,3786)	2:109:B:LEU:H	1:11:A:TYR:HD1	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3503)	1:59:A:LEU:HD11	2:159:B:ILE:HG13	2	0.85
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	2	0.85
(2,3428)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	2	0.85
(2,3427)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	2	0.85
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	6	0.85
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD13	10	0.85
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	2	0.85
(2,2488)	1:51:A:LEU:HB3	1:47:A:PHE:HD2	4	0.85
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG13	9	0.85
(2,1658)	2:111:B:ALA:HB2	2:151:B:ILE:HG13	9	0.85
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	1	0.85
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	2	0.85
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	7	0.85
(2,1132)	2:143:B:ILE:HA	2:146:B:LEU:HD12	8	0.85
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	2	0.84
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	1	0.84
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	7	0.84
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	2	0.84
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	1	0.84
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	1	0.84
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	5	0.84
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	10	0.84
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	10	0.84
(2,3173)	2:154:B:VAL:HG21	2:151:B:ILE:HG12	3	0.84
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	6	0.84
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG11	7	0.84
(2,2181)	1:17:A:HIS:HB2	1:56:A:ILE:HG23	4	0.84
(2,2151)	1:15:A:ILE:HG23	1:14:A:LEU:H	10	0.84
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	5	0.84
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	10	0.84
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	5	0.84
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	10	0.84
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD13	3	0.84
(2,1658)	2:111:B:ALA:HB2	2:151:B:ILE:HG13	5	0.84
(2,1266)	1:1:A:MET:HG3	2:152:B:GLU:HG3	2	0.84
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD11	5	0.84
(2,856)	2:111:B:ALA:HB2	2:107:B:TYR:HD1	5	0.84
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	5	0.84
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG22	9	0.84
(2,470)	1:22:A:THR:HG23	1:27:A:LYS:HD2	5	0.84
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	5	0.83
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	5	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	5	0.83
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	8	0.83
(2,3834)	2:121:B:LYS:H	2:121:B:LYS:HB3	6	0.83
(2,3739)	1:59:A:LEU:H	1:58:A:SER:HB3	5	0.83
(2,3496)	2:156:B:ALA:HB2	1:7:A:LEU:HB2	3	0.83
(2,3496)	2:156:B:ALA:HB3	1:7:A:LEU:HB2	8	0.83
(2,3175)	2:154:B:VAL:H	2:154:B:VAL:HG23	3	0.83
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	8	0.83
(2,3099)	2:146:B:LEU:HD23	2:149:B:LYS:HE3	2	0.83
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB2	8	0.83
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD21	5	0.83
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	3	0.83
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	3	0.83
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	3	0.83
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	7	0.83
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	9	0.83
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	2	0.82
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	3	0.82
(2,4414)	2:105:B:ALA:HA	2:108:B:LEU:HB3	8	0.82
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	4	0.82
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	9	0.82
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	3	0.82
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	5	0.82
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	7	0.82
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.82
(2,3962)	2:144:B:SER:H	2:143:B:ILE:HG12	3	0.82
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	4	0.82
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	6	0.82
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	7	0.82
(2,3515)	2:155:B:ILE:HG13	1:7:A:LEU:HD23	8	0.82
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG13	3	0.82
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	5	0.82
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	10	0.82
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG12	7	0.82
(2,3316)	1:8:A:ALA:HB1	2:112:B:LEU:HD21	9	0.82
(2,3300)	1:2:A:ALA:HB3	2:152:B:GLU:HG3	10	0.82
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	8	0.82
(2,3021)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	6	0.82
(2,2685)	2:105:B:ALA:HB2	2:108:B:LEU:HD22	5	0.82
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG13	5	0.82
(2,2412)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	8	0.82
(2,2181)	1:17:A:HIS:HB2	1:56:A:ILE:HG23	9	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	7	0.82
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	8	0.82
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	2	0.82
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	1	0.82
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	10	0.82
(2,1898)	2:146:B:LEU:HD11	2:151:B:ILE:HG13	8	0.82
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD13	1	0.82
(2,1700)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	0.82
(2,1648)	2:109:B:LEU:HA	2:109:B:LEU:HD13	4	0.82
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	3	0.82
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	9	0.82
(2,1251)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	0.82
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB2	1	0.82
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB2	3	0.82
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	5	0.81
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	10	0.81
(2,4222)	1:4:A:VAL:HB	1:3:A:SER:HB3	5	0.81
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	2	0.81
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	10	0.81
(2,4084)	2:124:B:LYS:HA	2:124:B:LYS:HD2	5	0.81
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	1	0.81
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	2	0.81
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	4	0.81
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	6	0.81
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	8	0.81
(2,4048)	1:59:A:LEU:HB3	1:59:A:LEU:HG	9	0.81
(2,4008)	1:4:A:VAL:HB	1:3:A:SER:HB3	5	0.81
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	3	0.81
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	5	0.81
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	10	0.81
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	8	0.81
(2,3456)	2:126:B:ILE:HD12	1:37:A:VAL:HG12	6	0.81
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	7	0.81
(2,3351)	1:16:A:LEU:HD11	2:130:B:VAL:HA	9	0.81
(2,3173)	2:154:B:VAL:HG21	2:151:B:ILE:HG12	9	0.81
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB2	1	0.81
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB2	2	0.81
(2,2810)	2:119:B:SER:HB3	2:120:B:ALA:HB1	2	0.81
(2,2721)	2:110:B:ALA:HB1	2:119:B:SER:H	2	0.81
(2,2181)	1:17:A:HIS:HB2	1:56:A:ILE:HG23	6	0.81
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	2	0.81
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	6	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	8	0.81
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	2	0.81
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	6	0.81
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	8	0.81
(2,1658)	2:111:B:ALA:HB2	2:151:B:ILE:HG13	2	0.81
(2,1393)	1:24:A:THR:HG21	1:26:A:ASP:HB3	1	0.81
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	10	0.81
(2,1371)	1:22:A:THR:HA	1:22:A:THR:HG21	6	0.81
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB2	6	0.81
(2,1173)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	10	0.81
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	5	0.8
(2,3962)	2:144:B:SER:H	2:143:B:ILE:HG12	4	0.8
(2,3739)	1:59:A:LEU:H	1:58:A:SER:HB3	8	0.8
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	6	0.8
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	3	0.8
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB2	3	0.8
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	7	0.8
(2,2974)	2:134:B:ALA:HB3	2:124:B:LYS:HE2	6	0.8
(2,2721)	2:110:B:ALA:HB2	2:119:B:SER:H	4	0.8
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	10	0.8
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG11	1	0.8
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG12	8	0.8
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG11	10	0.8
(2,2181)	1:17:A:HIS:HB3	1:56:A:ILE:HG23	3	0.8
(2,1745)	2:134:B:ALA:HB3	2:124:B:LYS:HE2	6	0.8
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG11	10	0.8
(2,1393)	1:24:A:THR:HG22	1:26:A:ASP:HB3	4	0.8
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	2	0.8
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	8	0.8
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	4	0.8
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB1	3	0.8
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB1	4	0.8
(2,1173)	2:154:B:VAL:HG11	2:146:B:LEU:HD21	2	0.8
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	2	0.8
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG21	2	0.8
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG21	8	0.8
(2,4222)	1:4:A:VAL:HB	1:3:A:SER:HB3	10	0.79
(2,4008)	1:4:A:VAL:HB	1:3:A:SER:HB3	10	0.79
(2,3962)	2:144:B:SER:H	2:143:B:ILE:HG12	1	0.79
(2,3962)	2:144:B:SER:H	2:143:B:ILE:HG12	10	0.79
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	2	0.79
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB3	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB2	7	0.79
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB2	9	0.79
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB2	10	0.79
(2,3166)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	8	0.79
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	2	0.79
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	5	0.79
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD22	6	0.79
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	9	0.79
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	4	0.79
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD13	5	0.79
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD12	10	0.79
(2,1542)	1:51:A:LEU:HD23	1:56:A:ILE:HB	3	0.79
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.79
(2,1393)	1:24:A:THR:HG23	1:26:A:ASP:HB3	8	0.79
(2,438)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	8	0.79
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	8	0.79
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG21	6	0.79
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG21	7	0.79
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG21	9	0.79
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD12	2	0.79
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG22	6	0.79
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	3	0.78
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	3	0.78
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	7	0.78
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	3	0.78
(2,3911)	2:133:B:GLU:H	2:133:B:GLU:HB3	2	0.78
(2,3021)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	2	0.78
(2,3017)	2:139:B:LEU:HD12	2:120:B:ALA:HA	2	0.78
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB3	6	0.78
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG2	3	0.78
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	7	0.78
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG12	4	0.78
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG13	6	0.78
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	3	0.78
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	9	0.78
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	4	0.78
(2,1809)	2:132:B:ILE:HG22	1:18:A:ASP:HB2	6	0.78
(2,1658)	2:111:B:ALA:HB3	2:151:B:ILE:HG13	10	0.78
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	7	0.78
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	2	0.78
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	3	0.78
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	3	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG2	3	0.78
(2,951)	2:125:B:LYS:HD3	2:129:B:SER:HB3	3	0.78
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	4	0.78
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	6	0.78
(2,847)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.78
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG11	10	0.78
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	2	0.78
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	7	0.78
(2,4140)	1:27:A:LYS:HA	1:27:A:LYS:HE2	2	0.77
(2,3857)	2:125:B:LYS:H	2:125:B:LYS:HE3	4	0.77
(2,3513)	2:155:B:ILE:HG23	1:11:A:TYR:HE2	1	0.77
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG13	10	0.77
(2,3393)	1:37:A:VAL:HG11	2:109:B:LEU:HD13	8	0.77
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	2	0.77
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	1	0.77
(2,3191)	2:156:B:ALA:HB3	2:153:B:ASP:HB2	4	0.77
(2,3173)	2:154:B:VAL:HG21	2:151:B:ILE:HG12	2	0.77
(2,2721)	2:110:B:ALA:HB2	2:119:B:SER:H	9	0.77
(2,2627)	2:101:B:MET:HE2	2:102:B:ARG:H	8	0.77
(2,2416)	1:40:A:GLU:HG3	1:39:A:VAL:HG12	2	0.77
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	2	0.77
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	5	0.77
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	4	0.77
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD12	8	0.77
(2,1608)	1:63:A:VAL:HA	1:63:A:VAL:HG22	4	0.77
(2,1393)	1:24:A:THR:HG23	1:26:A:ASP:HB3	2	0.77
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG21	5	0.77
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB1	8	0.77
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB3	10	0.77
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	7	0.77
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD23	1	0.77
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD22	3	0.77
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	2	0.77
(2,436)	1:16:A:LEU:HD11	1:27:A:LYS:HG3	1	0.77
(2,314)	2:153:B:ASP:H	2:151:B:ILE:HG22	9	0.77
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG21	5	0.77
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB2	10	0.77
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG12	1	0.77
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	1	0.76
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	1	0.76
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	8	0.76
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	9	0.76
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB2	2	0.76
(2,3151)	2:152:B:GLU:HB2	2:151:B:ILE:HG22	6	0.76
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	4	0.76
(2,2725)	2:111:B:ALA:HB2	2:107:B:TYR:HD1	5	0.76
(2,2721)	2:110:B:ALA:HB1	2:119:B:SER:H	6	0.76
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	1	0.76
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	9	0.76
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	4	0.76
(2,1898)	2:146:B:LEU:HD13	2:151:B:ILE:HG13	6	0.76
(2,1658)	2:111:B:ALA:HB1	2:151:B:ILE:HG13	7	0.76
(2,1608)	1:63:A:VAL:HA	1:63:A:VAL:HG22	9	0.76
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	1	0.76
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	7	0.76
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB2	2	0.76
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	8	0.76
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	4	0.76
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.76
(2,384)	1:10:A:ILE:HB	1:10:A:ILE:HD11	1	0.76
(2,384)	1:10:A:ILE:HB	1:10:A:ILE:HD11	3	0.76
(2,36)	1:13:A:ALA:H	1:51:A:LEU:HD13	8	0.76
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	8	0.75
(2,4170)	1:43:A:TRP:HA	1:46:A:LEU:HB2	3	0.75
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	3	0.75
(2,3857)	2:125:B:LYS:H	2:125:B:LYS:HE3	8	0.75
(2,3492)	2:152:B:GLU:HG3	1:7:A:LEU:HB3	9	0.75
(2,3388)	1:37:A:VAL:HG11	2:109:B:LEU:HD13	8	0.75
(2,2810)	2:119:B:SER:HB3	2:120:B:ALA:HB2	3	0.75
(2,2721)	2:110:B:ALA:HB2	2:119:B:SER:H	7	0.75
(2,2579)	1:61:A:CYS:HB3	1:62:A:ASN:HD21	5	0.75
(2,2181)	1:17:A:HIS:HB2	1:56:A:ILE:HG23	1	0.75
(2,2166)	1:16:A:LEU:HD11	1:27:A:LYS:HE3	9	0.75
(2,1898)	2:146:B:LEU:HD12	2:151:B:ILE:HG13	9	0.75
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	10	0.75
(2,1491)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	8	0.75
(2,1393)	1:24:A:THR:HG22	1:26:A:ASP:HB2	10	0.75
(2,1329)	1:14:A:LEU:HA	1:56:A:ILE:HG23	1	0.75
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	9	0.75
(2,1173)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	5	0.75
(2,1173)	2:154:B:VAL:HG13	2:146:B:LEU:HD21	9	0.75
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD22	6	0.75
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:51:A:LEU:HD13	1:47:A:PHE:HD2	6	0.75
(2,384)	1:10:A:ILE:HB	1:10:A:ILE:HD11	8	0.75
(2,314)	2:153:B:ASP:H	2:151:B:ILE:HG22	2	0.75
(2,31)	1:12:A:SER:H	2:109:B:LEU:HD22	3	0.75
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	7	0.74
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	9	0.74
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	9	0.74
(2,3857)	2:125:B:LYS:H	2:125:B:LYS:HE3	9	0.74
(2,3478)	2:132:B:ILE:HD11	1:19:A:ASP:HA	9	0.74
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	5	0.74
(2,3177)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	3	0.74
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	9	0.74
(2,2721)	2:110:B:ALA:HB2	2:119:B:SER:H	10	0.74
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	6	0.74
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB3	2	0.74
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	2	0.74
(2,2256)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	9	0.74
(2,2169)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	8	0.74
(2,2166)	1:16:A:LEU:HD11	1:27:A:LYS:HE3	4	0.74
(2,1898)	2:146:B:LEU:HD11	2:151:B:ILE:HG13	7	0.74
(2,1893)	2:146:B:LEU:HA	2:146:B:LEU:HD22	2	0.74
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	9	0.74
(2,1658)	2:111:B:ALA:HB2	2:151:B:ILE:HG13	4	0.74
(2,1620)	2:104:B:VAL:HA	2:146:B:LEU:HD23	1	0.74
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG21	9	0.74
(2,1374)	1:22:A:THR:HA	1:22:A:THR:HG21	6	0.74
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	2	0.74
(2,1056)	2:139:B:LEU:HD22	2:124:B:LYS:HA	3	0.74
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	2	0.74
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	8	0.74
(2,384)	1:10:A:ILE:HB	1:10:A:ILE:HD11	6	0.74
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	3	0.74
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	5	0.74
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	9	0.74
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	3	0.73
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	2	0.73
(2,3857)	2:125:B:LYS:H	2:125:B:LYS:HE3	6	0.73
(2,3440)	1:8:A:ALA:HA	2:109:B:LEU:HD12	4	0.73
(2,3173)	2:154:B:VAL:HG23	2:151:B:ILE:HG12	8	0.73
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG3	6	0.73
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD22	8	0.73
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD23	10	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2591)	1:63:A:VAL:HA	1:63:A:VAL:HG22	4	0.73
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	4	0.73
(2,1654)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	6	0.73
(2,1329)	1:14:A:LEU:HA	1:56:A:ILE:HG23	9	0.73
(2,1059)	2:139:B:LEU:HD12	2:120:B:ALA:HA	2	0.73
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG3	6	0.73
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	2	0.73
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE2	7	0.73
(2,386)	1:10:A:ILE:HD11	1:47:A:PHE:HE2	8	0.73
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD23	5	0.73
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG11	10	0.73
(2,4451)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	8	0.72
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	8	0.72
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	1	0.72
(2,4082)	2:123:B:ILE:HD12	2:107:B:TYR:HD2	8	0.72
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	4	0.72
(2,3464)	2:129:B:SER:HA	1:34:A:ALA:HA	2	0.72
(2,3428)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	9	0.72
(2,3427)	2:108:B:LEU:HD23	1:15:A:ILE:HD12	9	0.72
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	6	0.72
(2,3099)	2:146:B:LEU:HD12	2:149:B:LYS:HE3	10	0.72
(2,3021)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	7	0.72
(2,2810)	2:119:B:SER:HB3	2:120:B:ALA:HB1	8	0.72
(2,2640)	2:104:B:VAL:HA	2:146:B:LEU:HD23	1	0.72
(2,2579)	1:61:A:CYS:HB3	1:62:A:ASN:HD21	2	0.72
(2,2181)	1:17:A:HIS:HB2	1:56:A:ILE:HG23	8	0.72
(2,2069)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	6	0.72
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	1	0.72
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	1	0.72
(2,1944)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.72
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD12	7	0.72
(2,1654)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	5	0.72
(2,1542)	1:51:A:LEU:HD23	1:56:A:ILE:HB	2	0.72
(2,1056)	2:139:B:LEU:HD22	2:124:B:LYS:HA	2	0.72
(2,856)	2:111:B:ALA:HB1	2:107:B:TYR:HE1	10	0.72
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD23	5	0.72
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD23	7	0.72
(2,498)	1:25:A:GLU:HG3	1:48:A:ALA:HB1	8	0.72
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	8	0.72
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG11	9	0.72
(2,31)	1:12:A:SER:H	2:109:B:LEU:HD12	1	0.72
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4195)	2:149:B:LYS:HA	2:149:B:LYS:HD2	6	0.71
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	0.71
(2,3394)	1:37:A:VAL:HG13	2:109:B:LEU:HG	4	0.71
(2,3390)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	1	0.71
(2,3305)	1:4:A:VAL:HG23	2:112:B:LEU:HA	1	0.71
(2,3191)	2:156:B:ALA:HB1	2:153:B:ASP:HB2	5	0.71
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	3	0.71
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG3	8	0.71
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG3	9	0.71
(2,2746)	2:112:B:LEU:HD22	1:7:A:LEU:HG	1	0.71
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	2	0.71
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	5	0.71
(2,2591)	1:63:A:VAL:HA	1:63:A:VAL:HG22	9	0.71
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	5	0.71
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	7	0.71
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD23	1	0.71
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	3	0.71
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	7	0.71
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	6	0.71
(2,1919)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	8	0.71
(2,1893)	2:146:B:LEU:HA	2:146:B:LEU:HD22	7	0.71
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	1	0.71
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	3	0.71
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB1	7	0.71
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG3	8	0.71
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG3	9	0.71
(2,856)	2:111:B:ALA:HB1	2:107:B:TYR:HE1	1	0.71
(2,856)	2:111:B:ALA:HB2	2:107:B:TYR:HE1	7	0.71
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	5	0.71
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD21	10	0.71
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	7	0.71
(2,181)	2:107:B:TYR:H	2:146:B:LEU:HD13	10	0.71
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	3	0.7
(2,3464)	2:129:B:SER:HA	1:30:A:ALA:HA	9	0.7
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	5	0.7
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	6	0.7
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	5	0.7
(2,3103)	2:146:B:LEU:HA	2:146:B:LEU:HD22	2	0.7
(2,3021)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	3	0.7
(2,2810)	2:119:B:SER:HB3	2:120:B:ALA:HB1	4	0.7
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB3	7	0.7
(2,2722)	2:110:B:ALA:HB3	2:109:B:LEU:HB3	4	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD22	1	0.7
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	2	0.7
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	3	0.7
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	8	0.7
(2,1658)	2:111:B:ALA:HB2	2:151:B:ILE:HG13	6	0.7
(2,1614)	2:101:B:MET:HE2	1:14:A:LEU:HB2	8	0.7
(2,1608)	1:63:A:VAL:HA	1:63:A:VAL:HG11	10	0.7
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.7
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.7
(2,850)	2:110:B:ALA:HB2	2:118:B:PRO:HA	4	0.7
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	3	0.7
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	2	0.7
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	9	0.7
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	1	0.69
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	1	0.69
(2,3456)	2:126:B:ILE:HD13	1:37:A:VAL:HG13	1	0.69
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	9	0.69
(2,3296)	1:1:A:MET:HE3	2:156:B:ALA:HA	6	0.69
(2,3179)	2:154:B:VAL:HG11	2:155:B:ILE:H	8	0.69
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	2	0.69
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	2	0.69
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	2	0.69
(2,3099)	2:146:B:LEU:HD12	2:149:B:LYS:HE3	1	0.69
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB3	4	0.69
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB3	9	0.69
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	4	0.69
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HE1	6	0.69
(2,2716)	2:110:B:ALA:HB2	2:118:B:PRO:HA	4	0.69
(2,2494)	1:51:A:LEU:HD13	1:47:A:PHE:HD2	6	0.69
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD11	2	0.69
(2,2373)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	3	0.69
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	9	0.69
(2,2286)	1:28:A:ILE:HD12	1:44:A:PRO:HA	8	0.69
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	2	0.69
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD22	5	0.69
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD21	10	0.69
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	1	0.69
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	2	0.69
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	7	0.69
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	10	0.69
(2,1893)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.69
(2,1893)	2:146:B:LEU:HA	2:146:B:LEU:HD22	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1893)	2:146:B:LEU:HA	2:146:B:LEU:HD22	9	0.69
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	2	0.69
(2,1510)	1:28:A:ILE:HD12	1:44:A:PRO:HA	8	0.69
(2,1329)	1:14:A:LEU:HA	1:13:A:ALA:HB2	5	0.69
(2,1285)	1:4:A:VAL:HG22	1:7:A:LEU:HB3	4	0.69
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	7	0.69
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.69
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	8	0.69
(2,824)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	9	0.69
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD21	6	0.69
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	9	0.69
(2,522)	1:28:A:ILE:HD12	1:44:A:PRO:HA	8	0.69
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.69
(2,386)	1:10:A:ILE:HD13	1:47:A:PHE:HE2	2	0.69
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	10	0.69
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	10	0.68
(2,3496)	2:156:B:ALA:HB1	1:7:A:LEU:HB2	4	0.68
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD11	7	0.68
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	6	0.68
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	8	0.68
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	4	0.68
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	9	0.68
(2,3025)	2:139:B:LEU:HD22	2:124:B:LYS:HE3	6	0.68
(2,3021)	2:139:B:LEU:HD22	2:103:B:TYR:HE1	8	0.68
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG3	4	0.68
(2,2810)	2:119:B:SER:HB2	2:120:B:ALA:HB1	10	0.68
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB3	5	0.68
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	10	0.68
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	6	0.68
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	4	0.68
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	4	0.68
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	8	0.68
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	9	0.68
(2,1873)	2:143:B:ILE:HD11	2:142:B:VAL:HG12	10	0.68
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD12	9	0.68
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD3	2	0.68
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	4	0.68
(2,1032)	2:134:B:ALA:HB3	2:124:B:LYS:HE2	6	0.68
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG3	4	0.68
(2,850)	2:110:B:ALA:HB1	2:118:B:PRO:HA	8	0.68
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD21	8	0.68
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD22	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	6	0.68
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	10	0.68
(2,370)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	6	0.68
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	5	0.68
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	4	0.68
(2,206)	2:115:B:ASN:H	2:112:B:LEU:H	7	0.68
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	6	0.67
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	4	0.67
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	4	0.67
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	8	0.67
(2,3191)	2:156:B:ALA:HB2	2:153:B:ASP:HB2	8	0.67
(2,3179)	2:154:B:VAL:HG13	2:155:B:ILE:H	3	0.67
(2,3179)	2:154:B:VAL:HG12	2:155:B:ILE:H	9	0.67
(2,3171)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	7	0.67
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	5	0.67
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	3	0.67
(2,2878)	2:126:B:ILE:HA	2:125:B:LYS:HG3	7	0.67
(2,2810)	2:119:B:SER:HB2	2:120:B:ALA:HB1	9	0.67
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB2	6	0.67
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	8	0.67
(2,2721)	2:110:B:ALA:HB2	2:119:B:SER:H	3	0.67
(2,2716)	2:110:B:ALA:HB1	2:118:B:PRO:HA	8	0.67
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	4	0.67
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	8	0.67
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD2	6	0.67
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	4	0.67
(2,2166)	1:16:A:LEU:HD11	1:27:A:LYS:HE2	6	0.67
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	6	0.67
(2,2140)	1:14:A:LEU:HG	1:14:A:LEU:HD12	9	0.67
(2,2071)	1:7:A:LEU:HD22	1:11:A:TYR:HE1	10	0.67
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	5	0.67
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	1	0.67
(2,1873)	2:143:B:ILE:HD12	2:142:B:VAL:HG11	4	0.67
(2,1658)	2:111:B:ALA:HB3	2:151:B:ILE:HG13	3	0.67
(2,1542)	1:51:A:LEU:HD21	1:56:A:ILE:HB	7	0.67
(2,1541)	1:51:A:LEU:HD21	1:56:A:ILE:HD11	6	0.67
(2,1376)	1:23:A:VAL:HA	1:22:A:THR:HG22	6	0.67
(2,1172)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	7	0.67
(2,958)	2:126:B:ILE:HA	2:125:B:LYS:HG3	7	0.67
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	4	0.67
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE3	8	0.67
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD2	6	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	3	0.67
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	1	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	2	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	3	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	4	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	5	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	7	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	8	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	9	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.66
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	5	0.66
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	6	0.66
(2,3857)	2:125:B:LYS:H	2:125:B:LYS:HE3	2	0.66
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	4	0.66
(2,3171)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	5	0.66
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	2	0.66
(2,3103)	2:146:B:LEU:HA	2:146:B:LEU:HD22	7	0.66
(2,3006)	2:138:B:ARG:HD2	2:137:B:ASP:HB2	9	0.66
(2,2721)	2:110:B:ALA:HB2	2:119:B:SER:H	1	0.66
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	7	0.66
(2,2627)	2:101:B:MET:HE1	2:102:B:ARG:H	9	0.66
(2,2593)	1:63:A:VAL:HA	1:63:A:VAL:HG22	4	0.66
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB3	6	0.66
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	8	0.66
(2,2339)	1:33:A:LYS:H	1:33:A:LYS:HG3	9	0.66
(2,2337)	1:33:A:LYS:H	1:33:A:LYS:HG3	9	0.66
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	1	0.66
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	3	0.66
(2,1898)	2:146:B:LEU:HD13	2:151:B:ILE:HG13	2	0.66
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	3	0.66
(2,1542)	1:51:A:LEU:HD21	1:56:A:ILE:HB	5	0.66
(2,1172)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	5	0.66
(2,856)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	3	0.66
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	1	0.66
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB1	5	0.66
(2,4374)	1:59:A:LEU:HB3	1:59:A:LEU:HG	6	0.65
(2,3464)	2:129:B:SER:HA	1:34:A:ALA:HA	1	0.65
(2,3464)	2:129:B:SER:HA	1:34:A:ALA:HA	3	0.65
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.65
(2,3171)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	9	0.65
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	5	0.65
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	7	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3103)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.65
(2,3096)	2:146:B:LEU:HD22	2:142:B:VAL:HA	9	0.65
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD13	8	0.65
(2,2965)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	6	0.65
(2,2959)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	6	0.65
(2,2810)	2:119:B:SER:HB2	2:120:B:ALA:HB1	7	0.65
(2,2746)	2:112:B:LEU:HD21	1:7:A:LEU:HG	3	0.65
(2,2593)	1:63:A:VAL:HA	1:63:A:VAL:HG22	9	0.65
(2,2591)	1:63:A:VAL:HA	1:63:A:VAL:HG11	10	0.65
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	8	0.65
(2,2019)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	6	0.65
(2,1898)	2:146:B:LEU:HD12	2:151:B:ILE:HG13	5	0.65
(2,1804)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	8	0.65
(2,1800)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	8	0.65
(2,1794)	2:130:B:VAL:HG23	2:132:B:ILE:HD13	8	0.65
(2,1172)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	9	0.65
(2,1054)	2:139:B:LEU:HD22	2:124:B:LYS:HE3	6	0.65
(2,1017)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	6	0.65
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD22	4	0.65
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB3	5	0.65
(2,498)	1:25:A:GLU:HG3	1:48:A:ALA:HB1	6	0.65
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	1	0.65
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	2	0.65
(2,386)	1:10:A:ILE:HD11	1:47:A:PHE:HE2	6	0.65
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG13	5	0.65
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB1	3	0.65
(2,4456)	2:124:B:LYS:HA	2:124:B:LYS:HD2	5	0.64
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	4	0.64
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	8	0.64
(2,4080)	2:122:B:ASP:HA	2:125:B:LYS:HB2	5	0.64
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	5	0.64
(2,3503)	1:59:A:LEU:HD12	2:159:B:ILE:HG12	9	0.64
(2,3464)	2:129:B:SER:HA	1:30:A:ALA:HA	6	0.64
(2,3298)	1:1:A:MET:HG3	2:153:B:ASP:HB3	6	0.64
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	1	0.64
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	9	0.64
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	10	0.64
(2,3103)	2:146:B:LEU:HA	2:146:B:LEU:HD22	8	0.64
(2,3103)	2:146:B:LEU:HA	2:146:B:LEU:HD22	9	0.64
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	7	0.64
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.64
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.64
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.64
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.64
(2,2581)	1:61:A:CYS:HB3	1:60:A:ILE:H	1	0.64
(2,2571)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	6	0.64
(2,2346)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	4	0.64
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	1	0.64
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	5	0.64
(2,2095)	1:10:A:ILE:HD11	1:9:A:CYS:H	2	0.64
(2,1542)	1:51:A:LEU:HD22	1:56:A:ILE:HB	4	0.64
(2,846)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.64
(2,659)	1:46:A:LEU:H	1:46:A:LEU:HD23	2	0.64
(2,567)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	4	0.64
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	2	0.64
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	7	0.64
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	4	0.64
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD12	7	0.64
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD21	10	0.64
(2,117)	1:43:A:TRP:H	1:40:A:GLU:HG2	4	0.64
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG12	2	0.64
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	5	0.63
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	6	0.63
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	10	0.63
(2,3502)	2:159:B:ILE:HD11	1:60:A:ILE:HG13	10	0.63
(2,3496)	2:156:B:ALA:HB1	1:7:A:LEU:HB2	6	0.63
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	2	0.63
(2,3179)	2:154:B:VAL:HG13	2:155:B:ILE:H	2	0.63
(2,3171)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	6	0.63
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD22	6	0.63
(2,2945)	2:132:B:ILE:HD13	2:133:B:GLU:H	7	0.63
(2,2810)	2:119:B:SER:HB2	2:120:B:ALA:HB1	1	0.63
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.63
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.63
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB3	8	0.63
(2,2725)	2:111:B:ALA:HB1	2:107:B:TYR:HE1	10	0.63
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD23	4	0.63
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD21	9	0.63
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	4	0.63
(2,2339)	1:33:A:LYS:H	1:33:A:LYS:HG3	4	0.63
(2,2337)	1:33:A:LYS:H	1:33:A:LYS:HG3	4	0.63
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	7	0.63
(2,2282)	1:27:A:LYS:HG2	1:27:A:LYS:H	9	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	10	0.63
(2,2088)	1:10:A:ILE:HB	1:10:A:ILE:HD11	3	0.63
(2,2071)	1:7:A:LEU:HD21	1:11:A:TYR:HE1	1	0.63
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD13	2	0.63
(2,1716)	2:121:B:LYS:HG2	2:121:B:LYS:HE2	6	0.63
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	1	0.63
(2,1172)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	6	0.63
(2,850)	2:110:B:ALA:HB1	2:118:B:PRO:HA	2	0.63
(2,847)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	6	0.63
(2,586)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	3	0.63
(2,493)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	2	0.63
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	5	0.63
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD11	5	0.63
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD12	6	0.63
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	3	0.62
(2,3373)	1:34:A:ALA:HB2	2:125:B:LYS:HE2	7	0.62
(2,3179)	2:154:B:VAL:HG12	2:155:B:ILE:H	5	0.62
(2,3171)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	8	0.62
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	4	0.62
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	7	0.62
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	1	0.62
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	7	0.62
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.62
(2,2810)	2:119:B:SER:HB2	2:120:B:ALA:HB1	6	0.62
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.62
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.62
(2,2725)	2:111:B:ALA:HB1	2:107:B:TYR:HE1	1	0.62
(2,2725)	2:111:B:ALA:HB2	2:107:B:TYR:HE1	7	0.62
(2,2716)	2:110:B:ALA:HB1	2:118:B:PRO:HA	2	0.62
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.62
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD13	5	0.62
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	4	0.62
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	6	0.62
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	7	0.62
(2,2341)	1:34:A:ALA:HB2	2:125:B:LYS:HE2	7	0.62
(2,2339)	1:33:A:LYS:H	1:33:A:LYS:HG3	2	0.62
(2,2337)	1:33:A:LYS:H	1:33:A:LYS:HG3	2	0.62
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	3	0.62
(2,2095)	1:10:A:ILE:HD11	1:9:A:CYS:H	7	0.62
(2,2088)	1:10:A:ILE:HB	1:10:A:ILE:HD11	1	0.62
(2,2088)	1:10:A:ILE:HB	1:10:A:ILE:HD11	8	0.62
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	8	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1285)	1:4:A:VAL:HG21	1:7:A:LEU:HB3	10	0.62
(2,1172)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	8	0.62
(2,1056)	2:139:B:LEU:HD21	2:124:B:LYS:HA	6	0.62
(2,847)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	5	0.62
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	4	0.62
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.62
(2,619)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	6	0.62
(2,569)	1:34:A:ALA:HB2	2:125:B:LYS:HE2	7	0.62
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE3	10	0.62
(2,421)	1:15:A:ILE:HD13	2:106:B:SER:HA	4	0.62
(2,242)	2:125:B:LYS:H	2:125:B:LYS:HG2	1	0.62
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB3	7	0.62
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG22	2	0.62
(2,117)	1:43:A:TRP:H	1:40:A:GLU:HG2	6	0.62
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB2	5	0.62
(2,4533)	2:151:B:ILE:HD13	2:150:B:ASN:H	8	0.61
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	4	0.61
(2,3855)	2:124:B:LYS:H	2:124:B:LYS:HD2	5	0.61
(2,3492)	2:152:B:GLU:HG3	1:7:A:LEU:HB3	2	0.61
(2,3179)	2:154:B:VAL:HG12	2:155:B:ILE:H	7	0.61
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	10	0.61
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD12	2	0.61
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD11	9	0.61
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	9	0.61
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.61
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.61
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.61
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.61
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.61
(2,2775)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.61
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD23	2	0.61
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	1	0.61
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	2	0.61
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	5	0.61
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	7	0.61
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	8	0.61
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	10	0.61
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	2	0.61
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	4	0.61
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	5	0.61
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	6	0.61
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	7	0.61
(2,1285)	1:4:A:VAL:HG23	1:7:A:LEU:HB3	1	0.61
(2,1285)	1:4:A:VAL:HG23	1:7:A:LEU:HB3	5	0.61
(2,1285)	1:4:A:VAL:HG22	1:7:A:LEU:HB3	6	0.61
(2,1175)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.61
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG21	9	0.61
(2,555)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	6	0.61
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD13	2	0.61
(2,242)	2:125:B:LYS:H	2:125:B:LYS:HG2	2	0.61
(2,242)	2:125:B:LYS:H	2:125:B:LYS:HG2	10	0.61
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	3	0.61
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	5	0.61
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	6	0.61
(2,159)	1:63:A:VAL:H	1:62:A:ASN:HB2	3	0.61
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG13	4	0.61
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB1	7	0.61
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	2	0.6
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	7	0.6
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	6	0.6
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD11	2	0.6
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD11	9	0.6
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	3	0.6
(2,3305)	1:4:A:VAL:HG23	2:112:B:LEU:HA	9	0.6
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	5	0.6
(2,3171)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	2	0.6
(2,3171)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	4	0.6
(2,3166)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	6	0.6
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.6
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	1	0.6
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	10	0.6
(2,3099)	2:146:B:LEU:HD12	2:149:B:LYS:HE3	6	0.6
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.6
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.6
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD23	7	0.6
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	2	0.6
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD13	3	0.6
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	3	0.6
(2,2438)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	9	0.6
(2,2346)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	8	0.6
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	3	0.6
(2,2095)	1:10:A:ILE:HD11	1:47:A:PHE:HE2	1	0.6
(2,2095)	1:10:A:ILE:HD11	1:9:A:CYS:H	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2088)	1:10:A:ILE:HB	1:10:A:ILE:HD11	6	0.6
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	0.6
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG2	1	0.6
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	5	0.6
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	4	0.6
(2,1383)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	8	0.6
(2,1266)	1:1:A:MET:HG2	2:152:B:GLU:HG3	6	0.6
(2,1172)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	2	0.6
(2,1172)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	4	0.6
(2,1132)	2:146:B:LEU:HD22	2:142:B:VAL:HA	9	0.6
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	2	0.6
(2,619)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	4	0.6
(2,567)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	8	0.6
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	3	0.6
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	4	0.6
(2,386)	1:10:A:ILE:HD11	1:47:A:PHE:HE2	1	0.6
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD11	8	0.6
(2,206)	2:115:B:ASN:H	2:111:B:ALA:H	1	0.6
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG13	1	0.6
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB3	10	0.6
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	4	0.59
(2,4462)	2:125:B:LYS:H	2:125:B:LYS:HB2	5	0.59
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	2	0.59
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	5	0.59
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD11	5	0.59
(2,3492)	2:152:B:GLU:HG3	1:7:A:LEU:HB3	4	0.59
(2,3460)	1:35:A:ALA:HB1	2:126:B:ILE:HG23	2	0.59
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	9	0.59
(2,3385)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	3	0.59
(2,3305)	1:4:A:VAL:HG22	2:112:B:LEU:HA	7	0.59
(2,3171)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	1	0.59
(2,3171)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	10	0.59
(2,3142)	2:151:B:ILE:HD13	2:150:B:ASN:HA	8	0.59
(2,2810)	2:119:B:SER:HB2	2:120:B:ALA:HB1	5	0.59
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.59
(2,2746)	2:112:B:LEU:HD21	1:7:A:LEU:HG	7	0.59
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	5	0.59
(2,2095)	1:10:A:ILE:HD11	1:9:A:CYS:H	9	0.59
(2,2095)	1:10:A:ILE:HD11	1:9:A:CYS:H	10	0.59
(2,2072)	1:7:A:LEU:HD11	1:7:A:LEU:H	6	0.59
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	7	0.59
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1873)	2:143:B:ILE:HD11	2:142:B:VAL:HG11	1	0.59
(2,1873)	2:143:B:ILE:HD12	2:142:B:VAL:HG11	3	0.59
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD11	5	0.59
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD12	6	0.59
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD13	7	0.59
(2,1659)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	9	0.59
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	5	0.59
(2,1172)	2:154:B:VAL:HG23	2:107:B:TYR:HE1	1	0.59
(2,1172)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	10	0.59
(2,850)	2:110:B:ALA:HB1	2:118:B:PRO:HA	6	0.59
(2,558)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	8	0.59
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE3	5	0.59
(2,357)	1:4:A:VAL:HG23	2:112:B:LEU:HA	1	0.59
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG2	1	0.59
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG23	7	0.59
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB1	9	0.59
(2,4291)	1:26:A:ASP:HB3	1:26:A:ASP:H	3	0.58
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	2	0.58
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	10	0.58
(2,3431)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	8	0.58
(2,3364)	1:31:A:LEU:HD11	2:130:B:VAL:HA	2	0.58
(2,3168)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.58
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	10	0.58
(2,3017)	2:139:B:LEU:HD12	2:120:B:ALA:HA	6	0.58
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	1	0.58
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	2	0.58
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	5	0.58
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	6	0.58
(2,2982)	2:134:B:ALA:HB3	2:124:B:LYS:HA	8	0.58
(2,2889)	2:126:B:ILE:HD12	2:109:B:LEU:HB3	4	0.58
(2,2808)	2:119:B:SER:HB3	2:121:B:LYS:HD3	4	0.58
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.58
(2,2776)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.58
(2,2716)	2:110:B:ALA:HB1	2:118:B:PRO:HA	6	0.58
(2,2627)	2:101:B:MET:HE1	2:102:B:ARG:H	4	0.58
(2,2593)	1:63:A:VAL:HA	1:63:A:VAL:HG11	10	0.58
(2,2579)	1:61:A:CYS:HB3	1:62:A:ASN:HD21	8	0.58
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD11	7	0.58
(2,2095)	1:10:A:ILE:HD12	1:9:A:CYS:H	3	0.58
(2,2095)	1:10:A:ILE:HD11	1:9:A:CYS:H	4	0.58
(2,2095)	1:10:A:ILE:HD12	1:9:A:CYS:H	6	0.58
(2,1980)	2:159:B:ILE:HA	2:159:B:ILE:HD13	3	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	4	0.58
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	7	0.58
(2,1700)	2:139:B:LEU:HD12	2:120:B:ALA:HA	2	0.58
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.58
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	6	0.58
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	9	0.58
(2,1542)	1:51:A:LEU:HD22	1:56:A:ILE:HB	10	0.58
(2,1285)	1:4:A:VAL:HG22	1:7:A:LEU:HB3	8	0.58
(2,1272)	1:2:A:ALA:HB2	1:6:A:GLU:HB3	3	0.58
(2,1173)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	3	0.58
(2,1134)	2:146:B:LEU:HA	2:146:B:LEU:HD22	2	0.58
(2,1028)	2:134:B:ALA:HB3	2:124:B:LYS:HA	8	0.58
(2,964)	2:126:B:ILE:HD12	2:109:B:LEU:HB3	4	0.58
(2,850)	2:110:B:ALA:HB1	2:118:B:PRO:HA	5	0.58
(2,498)	1:25:A:GLU:HG3	1:48:A:ALA:HB3	7	0.58
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	6	0.58
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD22	4	0.58
(2,159)	1:63:A:VAL:H	1:62:A:ASN:HB2	1	0.58
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB1	2	0.58
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB3	1	0.58
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB2	2	0.58
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB2	6	0.58
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	1	0.57
(2,4291)	1:26:A:ASP:HB3	1:26:A:ASP:H	6	0.57
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	4	0.57
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	7	0.57
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	4	0.57
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	8	0.57
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	4	0.57
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	1	0.57
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	1	0.57
(2,3502)	2:159:B:ILE:HD11	1:60:A:ILE:HG13	1	0.57
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD11	3	0.57
(2,3492)	2:152:B:GLU:HG3	1:7:A:LEU:HB3	5	0.57
(2,3179)	2:154:B:VAL:HG11	2:155:B:ILE:H	6	0.57
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD11	7	0.57
(2,2746)	2:112:B:LEU:HD23	1:7:A:LEU:HG	6	0.57
(2,2725)	2:111:B:ALA:HB3	2:107:B:TYR:HD1	3	0.57
(2,2716)	2:110:B:ALA:HB1	2:118:B:PRO:HA	5	0.57
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD23	4	0.57
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	3	0.57
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	6	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2339)	1:33:A:LYS:H	1:33:A:LYS:HG3	5	0.57
(2,2337)	1:33:A:LYS:H	1:33:A:LYS:HG3	5	0.57
(2,2166)	1:16:A:LEU:HD21	1:27:A:LYS:HE3	1	0.57
(2,2166)	1:16:A:LEU:HD11	1:27:A:LYS:HE3	5	0.57
(2,2095)	1:10:A:ILE:HD12	1:9:A:CYS:H	8	0.57
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	1	0.57
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	10	0.57
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD13	2	0.57
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD11	8	0.57
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	8	0.57
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.57
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.57
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.57
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.57
(2,1659)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	3	0.57
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	1	0.57
(2,1285)	1:4:A:VAL:HG22	1:7:A:LEU:HB3	2	0.57
(2,1285)	1:4:A:VAL:HG21	1:7:A:LEU:HB3	3	0.57
(2,1283)	1:4:A:VAL:HG23	1:7:A:LEU:HD22	1	0.57
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD13	3	0.57
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	6	0.57
(2,555)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	3	0.57
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	10	0.57
(2,438)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	7	0.57
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD12	9	0.57
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG22	10	0.57
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD21	3	0.57
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG11	2	0.57
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB1	8	0.57
(2,4458)	2:125:B:LYS:HA	2:125:B:LYS:HB3	1	0.56
(2,4458)	2:125:B:LYS:HA	2:125:B:LYS:HB3	2	0.56
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	3	0.56
(2,4291)	1:26:A:ASP:HB3	1:26:A:ASP:H	7	0.56
(2,4290)	1:26:A:ASP:HB3	1:26:A:ASP:H	3	0.56
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	10	0.56
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	5	0.56
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	6	0.56
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	10	0.56
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	7	0.56
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	3	0.56
(2,3361)	1:31:A:LEU:HD13	2:129:B:SER:HA	3	0.56
(2,3361)	1:31:A:LEU:HD11	2:129:B:SER:HA	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3300)	1:2:A:ALA:HB1	2:152:B:GLU:HG3	6	0.56
(2,3179)	2:154:B:VAL:HG13	2:155:B:ILE:H	4	0.56
(2,3179)	2:154:B:VAL:HG13	2:155:B:ILE:H	10	0.56
(2,3171)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	3	0.56
(2,3106)	2:146:B:LEU:HD22	2:142:B:VAL:HA	9	0.56
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	8	0.56
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	10	0.56
(2,2965)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	8	0.56
(2,2959)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	8	0.56
(2,2921)	1:31:A:LEU:HD13	2:129:B:SER:HA	3	0.56
(2,2921)	1:31:A:LEU:HD11	2:129:B:SER:HA	9	0.56
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	4	0.56
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	9	0.56
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	7	0.56
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD12	9	0.56
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	2	0.56
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	4	0.56
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	7	0.56
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	10	0.56
(2,1872)	2:143:B:ILE:HB	2:143:B:ILE:HD12	9	0.56
(2,1851)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	0.56
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	2	0.56
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	3	0.56
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.56
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.56
(2,1614)	2:101:B:MET:HE2	1:14:A:LEU:HB2	3	0.56
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	8	0.56
(2,1542)	1:51:A:LEU:HD23	1:56:A:ILE:HB	9	0.56
(2,1393)	1:24:A:THR:HG22	1:26:A:ASP:HB2	6	0.56
(2,1172)	2:154:B:VAL:HG21	2:107:B:TYR:HE1	3	0.56
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	7	0.56
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	3	0.56
(2,1017)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	8	0.56
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	4	0.56
(2,850)	2:110:B:ALA:HB2	2:118:B:PRO:HA	9	0.56
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	1	0.56
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	5	0.56
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	7	0.56
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	7	0.56
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB1	9	0.56
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB2	10	0.56
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	7	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	2	0.55
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	3	0.55
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	4	0.55
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	10	0.55
(2,3857)	2:125:B:LYS:H	2:125:B:LYS:HE3	10	0.55
(2,3347)	1:15:A:ILE:HG23	2:101:B:MET:HE3	5	0.55
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	3	0.55
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	6	0.55
(2,2826)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	2	0.55
(2,2826)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	6	0.55
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	6	0.55
(2,2716)	2:110:B:ALA:HB2	2:118:B:PRO:HA	9	0.55
(2,2715)	2:110:B:ALA:HB1	2:115:B:ASN:H	4	0.55
(2,2600)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	8	0.55
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD12	10	0.55
(2,2339)	1:33:A:LYS:H	1:33:A:LYS:HG3	10	0.55
(2,2337)	1:33:A:LYS:H	1:33:A:LYS:HG3	10	0.55
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	5	0.55
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	8	0.55
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	9	0.55
(2,1994)	2:161:B:LYS:HE3	2:161:B:LYS:HB2	10	0.55
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	9	0.55
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	6	0.55
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.55
(2,1659)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	4	0.55
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD12	7	0.55
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	6	0.55
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	6	0.55
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD13	1	0.55
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	6	0.55
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	8	0.55
(2,760)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	9	0.55
(2,682)	1:50:A:ALA:HB3	1:46:A:LEU:HB3	4	0.55
(2,493)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	5	0.55
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	9	0.55
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG22	1	0.55
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG22	2	0.55
(2,32)	1:12:A:SER:H	1:13:A:ALA:HB1	4	0.55
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	9	0.54
(2,4291)	1:26:A:ASP:HB3	1:26:A:ASP:H	10	0.54
(2,4290)	1:26:A:ASP:HB3	1:26:A:ASP:H	6	0.54
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	9	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	5	0.54
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	5	0.54
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	6	0.54
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	8	0.54
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	10	0.54
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	2	0.54
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	9	0.54
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	9	0.54
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	7	0.54
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	0.54
(2,3416)	2:101:B:MET:HE1	1:17:A:HIS:HD2	1	0.54
(2,3361)	1:31:A:LEU:HD11	2:129:B:SER:HA	1	0.54
(2,3296)	1:1:A:MET:HE2	2:156:B:ALA:HA	4	0.54
(2,3177)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	1	0.54
(2,3162)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.54
(2,3123)	2:147:B:ASN:HB2	2:148:B:GLY:H	9	0.54
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.54
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.54
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	3	0.54
(2,2722)	2:110:B:ALA:HB1	2:109:B:LEU:HB3	9	0.54
(2,2715)	2:110:B:ALA:HB1	2:115:B:ASN:H	8	0.54
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD23	3	0.54
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	9	0.54
(2,2412)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	6	0.54
(2,2373)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	1	0.54
(2,2258)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	1	0.54
(2,2072)	1:7:A:LEU:HD11	1:7:A:LEU:H	4	0.54
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	3	0.54
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG11	9	0.54
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	8	0.54
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD13	6	0.54
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	10	0.54
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.54
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.54
(2,1675)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.54
(2,1134)	2:146:B:LEU:HA	2:146:B:LEU:HD22	7	0.54
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.54
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	7	0.54
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	5	0.54
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	8	0.54
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.54
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.54
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.54
(2,792)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	5	0.54
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	2	0.54
(2,558)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	4	0.54
(2,555)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	4	0.54
(2,468)	1:22:A:THR:HA	1:22:A:THR:HG21	6	0.54
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG22	4	0.54
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD1	10	0.54
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD23	5	0.54
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD23	6	0.54
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD22	8	0.54
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	2	0.53
(2,4290)	1:26:A:ASP:HB3	1:26:A:ASP:H	7	0.53
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	9	0.53
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	7	0.53
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.53
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	2	0.53
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	3	0.53
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	2	0.53
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	2	0.53
(2,3503)	1:59:A:LEU:HD11	2:159:B:ILE:HG12	1	0.53
(2,3493)	2:152:B:GLU:HG3	1:4:A:VAL:HB	6	0.53
(2,3172)	2:154:B:VAL:HG11	2:155:B:ILE:H	8	0.53
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	3	0.53
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	9	0.53
(2,2850)	2:123:B:ILE:HG23	2:139:B:LEU:HA	4	0.53
(2,2722)	2:110:B:ALA:HB1	2:109:B:LEU:HB3	1	0.53
(2,2715)	2:110:B:ALA:HB1	2:115:B:ASN:H	5	0.53
(2,2715)	2:110:B:ALA:HB1	2:115:B:ASN:H	6	0.53
(2,2583)	1:61:A:CYS:HB2	1:65:A:ALA:HB1	10	0.53
(2,2421)	1:41:A:PRO:HA	1:39:A:VAL:HG21	1	0.53
(2,2412)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	4	0.53
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	5	0.53
(2,2258)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	4	0.53
(2,2072)	1:7:A:LEU:HD12	1:7:A:LEU:H	2	0.53
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	7	0.53
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	8	0.53
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	2	0.53
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	4	0.53
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	5	0.53
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	9	0.53
(2,1842)	2:139:B:LEU:HD12	2:120:B:ALA:HA	3	0.53
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	2	0.53
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	5	0.53
(2,1351)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	8	0.53
(2,1341)	1:15:A:ILE:HD12	1:15:A:ILE:HB	4	0.53
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	1	0.53
(2,1134)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.53
(2,1134)	2:146:B:LEU:HA	2:146:B:LEU:HD22	9	0.53
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG21	8	0.53
(2,1059)	2:139:B:LEU:HD12	2:120:B:ALA:HA	6	0.53
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	9	0.53
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.53
(2,850)	2:110:B:ALA:HB2	2:118:B:PRO:HA	7	0.53
(2,341)	1:1:A:MET:HG2	1:7:A:LEU:HD22	3	0.53
(2,291)	2:143:B:ILE:H	2:143:B:ILE:HG23	3	0.53
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	1	0.53
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	4	0.53
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD23	10	0.53
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG13	3	0.53
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG22	5	0.53
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	1	0.52
(2,4521)	2:145:B:GLU:HG2	2:145:B:GLU:H	6	0.52
(2,4458)	2:125:B:LYS:HA	2:125:B:LYS:HB3	10	0.52
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	8	0.52
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	2	0.52
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	4	0.52
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	8	0.52
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	9	0.52
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	9	0.52
(2,3380)	1:35:A:ALA:HB1	2:126:B:ILE:HA	2	0.52
(2,3361)	1:31:A:LEU:HD12	2:129:B:SER:HA	6	0.52
(2,3131)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	8	0.52
(2,3123)	2:147:B:ASN:HB2	2:148:B:GLY:H	2	0.52
(2,3032)	2:140:B:ASN:HA	2:143:B:ILE:HD13	5	0.52
(2,3025)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	2	0.52
(2,3025)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	4	0.52
(2,2950)	2:132:B:ILE:HD13	2:130:B:VAL:H	1	0.52
(2,2826)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	9	0.52
(2,2722)	2:110:B:ALA:HB1	2:109:B:LEU:HB3	7	0.52
(2,2716)	2:110:B:ALA:HB2	2:118:B:PRO:HA	7	0.52
(2,2714)	2:110:B:ALA:HB3	2:123:B:ILE:H	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2685)	2:105:B:ALA:HB3	2:108:B:LEU:HD23	9	0.52
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	9	0.52
(2,2169)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	7	0.52
(2,2094)	1:10:A:ILE:HD13	1:7:A:LEU:H	1	0.52
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	2	0.52
(2,2020)	2:166:B:PRO:HB3	2:166:B:PRO:HD3	6	0.52
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	10	0.52
(2,1716)	2:121:B:LYS:HG2	2:121:B:LYS:HE2	1	0.52
(2,1614)	2:101:B:MET:HE1	1:14:A:LEU:HB2	6	0.52
(2,1285)	1:4:A:VAL:HG21	1:7:A:LEU:HB3	7	0.52
(2,1283)	1:4:A:VAL:HG21	1:7:A:LEU:HD23	10	0.52
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	2	0.52
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	3	0.52
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	9	0.52
(2,1134)	2:146:B:LEU:HA	2:146:B:LEU:HD22	8	0.52
(2,1060)	2:139:B:LEU:HD22	2:124:B:LYS:HD2	6	0.52
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	4	0.52
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	6	0.52
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	7	0.52
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.52
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.52
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.52
(2,771)	1:11:A:TYR:HD1	2:108:B:LEU:HD22	3	0.52
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	10	0.52
(2,493)	1:25:A:GLU:HB3	1:48:A:ALA:HB1	10	0.52
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	6	0.52
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	7	0.52
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG23	3	0.52
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB3	3	0.52
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	10	0.52
(2,4520)	2:145:B:GLU:HG2	2:145:B:GLU:H	8	0.51
(2,4290)	1:26:A:ASP:HB3	1:26:A:ASP:H	10	0.51
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	2	0.51
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	3	0.51
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	7	0.51
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG23	7	0.51
(2,3373)	1:34:A:ALA:HB3	2:125:B:LYS:HE2	3	0.51
(2,3361)	1:31:A:LEU:HD11	2:129:B:SER:HA	2	0.51
(2,3361)	1:31:A:LEU:HD12	2:129:B:SER:HA	7	0.51
(2,3297)	1:1:A:MET:HE2	2:152:B:GLU:HA	1	0.51
(2,3296)	1:1:A:MET:HE2	2:156:B:ALA:HA	7	0.51
(2,3177)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	7	0.51
(2,3050)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.51
(2,3050)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.51
(2,2950)	2:132:B:ILE:HD13	2:130:B:VAL:H	2	0.51
(2,2950)	2:132:B:ILE:HD11	2:130:B:VAL:H	4	0.51
(2,2950)	2:132:B:ILE:HD11	2:130:B:VAL:H	7	0.51
(2,2950)	2:132:B:ILE:HD11	2:130:B:VAL:H	10	0.51
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB2	8	0.51
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB2	3	0.51
(2,2748)	2:112:B:LEU:H	2:112:B:LEU:HD12	1	0.51
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	4	0.51
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	8	0.51
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	10	0.51
(2,2341)	1:34:A:ALA:HB3	2:125:B:LYS:HE2	3	0.51
(2,2257)	1:25:A:GLU:HG3	1:29:A:ASN:HD22	9	0.51
(2,2072)	1:7:A:LEU:HD12	1:7:A:LEU:H	3	0.51
(2,2072)	1:7:A:LEU:HD11	1:7:A:LEU:H	10	0.51
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	7	0.51
(2,1898)	2:146:B:LEU:HD13	2:151:B:ILE:HG13	10	0.51
(2,1721)	2:122:B:ASP:HA	2:125:B:LYS:HG3	5	0.51
(2,1716)	2:121:B:LYS:HG2	2:121:B:LYS:HE2	3	0.51
(2,1659)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	2	0.51
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	3	0.51
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	10	0.51
(2,1341)	1:15:A:ILE:HD11	1:15:A:ILE:HB	3	0.51
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	2	0.51
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	10	0.51
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	5	0.51
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	8	0.51
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	10	0.51
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD13	5	0.51
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD12	10	0.51
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD11	4	0.51
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	2	0.51
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.51
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.51
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.51
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.51
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.51
(2,886)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.51
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	9	0.51
(2,569)	1:34:A:ALA:HB3	2:125:B:LYS:HE2	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	9	0.51
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	5	0.51
(2,426)	1:15:A:ILE:HG21	1:18:A:ASP:HB3	1	0.51
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	10	0.51
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	8	0.51
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE2	4	0.51
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	7	0.51
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	6	0.51
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG12	7	0.51
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG12	8	0.51
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG22	6	0.51
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB3	7	0.51
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	5	0.51
(2,4521)	2:145:B:GLU:HG2	2:145:B:GLU:H	5	0.5
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	1	0.5
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	6	0.5
(2,4080)	2:122:B:ASP:HA	2:125:B:LYS:HB2	10	0.5
(2,3836)	2:122:B:ASP:H	2:121:B:LYS:HB3	10	0.5
(2,3464)	2:129:B:SER:HA	1:30:A:ALA:HA	7	0.5
(2,3361)	1:31:A:LEU:HD11	2:129:B:SER:HA	5	0.5
(2,3305)	1:4:A:VAL:HG22	2:112:B:LEU:HA	3	0.5
(2,3172)	2:154:B:VAL:HG13	2:155:B:ILE:H	3	0.5
(2,3172)	2:154:B:VAL:HG12	2:155:B:ILE:H	9	0.5
(2,3170)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.5
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	9	0.5
(2,3050)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.5
(2,2921)	1:31:A:LEU:HD11	2:129:B:SER:HA	5	0.5
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	9	0.5
(2,2759)	2:116:B:SER:H	2:115:B:ASN:HB2	1	0.5
(2,2746)	2:112:B:LEU:HD23	1:7:A:LEU:HG	8	0.5
(2,2722)	2:110:B:ALA:HB3	2:109:B:LEU:HB3	8	0.5
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.5
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	4	0.5
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB3	7	0.5
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD13	4	0.5
(2,1974)	2:159:B:ILE:HA	2:159:B:ILE:HD13	3	0.5
(2,1941)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.5
(2,1864)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.5
(2,1864)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.5
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	1	0.5
(2,1654)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	4	0.5
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1393)	1:24:A:THR:HG22	1:26:A:ASP:HB2	7	0.5
(2,1341)	1:15:A:ILE:HD11	1:15:A:ILE:HB	6	0.5
(2,1285)	1:4:A:VAL:HG22	1:7:A:LEU:HB3	9	0.5
(2,1157)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	4	0.5
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB2	1	0.5
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB2	10	0.5
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	1	0.5
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	3	0.5
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	9	0.5
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.5
(2,850)	2:110:B:ALA:HB2	2:118:B:PRO:HA	10	0.5
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	3	0.5
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	3	0.5
(2,555)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	1	0.5
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	6	0.5
(2,391)	1:10:A:ILE:HG22	2:159:B:ILE:HG12	8	0.5
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	9	0.5
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	10	0.5
(2,181)	2:107:B:TYR:H	2:146:B:LEU:HD13	6	0.5
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD22	3	0.5
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD23	4	0.5
(2,31)	1:12:A:SER:H	2:109:B:LEU:HD12	10	0.5
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	8	0.5
(2,4462)	2:125:B:LYS:H	2:125:B:LYS:HB2	10	0.49
(2,4458)	2:125:B:LYS:HA	2:125:B:LYS:HB3	5	0.49
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	5	0.49
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	7	0.49
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	6	0.49
(2,4201)	2:155:B:ILE:HA	2:155:B:ILE:HG12	1	0.49
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	1	0.49
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	3	0.49
(2,4124)	2:159:B:ILE:HA	2:159:B:ILE:HG12	5	0.49
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	1	0.49
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	6	0.49
(2,3492)	2:152:B:GLU:HG3	1:7:A:LEU:HB3	10	0.49
(2,3340)	1:15:A:ILE:HD11	2:127:B:LEU:HB3	3	0.49
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	6	0.49
(2,3143)	2:151:B:ILE:HD12	2:108:B:LEU:HD12	8	0.49
(2,3123)	2:147:B:ASN:HB2	2:148:B:GLY:H	7	0.49
(2,2982)	2:134:B:ALA:HB1	2:124:B:LYS:HA	4	0.49
(2,2950)	2:132:B:ILE:HD13	2:130:B:VAL:H	3	0.49
(2,2950)	2:132:B:ILE:HD11	2:130:B:VAL:H	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	3	0.49
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	7	0.49
(2,2826)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	1	0.49
(2,2746)	2:112:B:LEU:HD22	1:7:A:LEU:HG	2	0.49
(2,2722)	2:110:B:ALA:HB1	2:109:B:LEU:HB3	3	0.49
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	6	0.49
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	3	0.49
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	10	0.49
(2,2328)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	8	0.49
(2,2072)	1:7:A:LEU:HD11	1:7:A:LEU:H	1	0.49
(2,2072)	1:7:A:LEU:HD12	1:7:A:LEU:H	5	0.49
(2,2072)	1:7:A:LEU:HD12	1:7:A:LEU:H	7	0.49
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	3	0.49
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	9	0.49
(2,1864)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.49
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD2	1	0.49
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	5	0.49
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	7	0.49
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	9	0.49
(2,1658)	2:111:B:ALA:HB3	2:151:B:ILE:HG13	1	0.49
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	3	0.49
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD13	5	0.49
(2,1391)	1:24:A:THR:HG23	1:27:A:LYS:HE3	5	0.49
(2,1350)	1:16:A:LEU:HD11	1:27:A:LYS:HG3	1	0.49
(2,1283)	1:4:A:VAL:HG22	1:7:A:LEU:HD21	4	0.49
(2,1159)	2:152:B:GLU:HA	2:155:B:ILE:HD12	9	0.49
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB2	6	0.49
(2,1102)	2:143:B:ILE:HD12	2:107:B:TYR:HD2	1	0.49
(2,1054)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	2	0.49
(2,1054)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	4	0.49
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD12	8	0.49
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG3	1	0.49
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	3	0.49
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	1	0.49
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.49
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.49
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.49
(2,846)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	6	0.49
(2,586)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	1	0.49
(2,558)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	5	0.49
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	7	0.49
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	2	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	7	0.49
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	4	0.49
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	10	0.49
(2,242)	2:125:B:LYS:H	2:125:B:LYS:HG2	5	0.49
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	7	0.49
(2,217)	2:117:B:SER:H	2:115:B:ASN:HD21	10	0.49
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD22	1	0.49
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD22	7	0.49
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	1	0.49
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	3	0.49
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	7	0.49
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	4	0.48
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	8	0.48
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	0.48
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	5	0.48
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	7	0.48
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	9	0.48
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	4	0.48
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	10	0.48
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	5	0.48
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	7	0.48
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	5	0.48
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	7	0.48
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	4	0.48
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	10	0.48
(2,3495)	2:156:B:ALA:HB3	1:7:A:LEU:HD13	8	0.48
(2,3270)	2:165:B:VAL:HG13	2:161:B:LYS:HG3	8	0.48
(2,3123)	2:147:B:ASN:HB3	2:148:B:GLY:H	1	0.48
(2,3054)	2:142:B:VAL:HG13	2:107:B:TYR:HD2	3	0.48
(2,3025)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	10	0.48
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	1	0.48
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	2	0.48
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	4	0.48
(2,2748)	2:112:B:LEU:H	2:112:B:LEU:HD12	3	0.48
(2,2746)	2:112:B:LEU:HD23	1:7:A:LEU:HG	10	0.48
(2,2716)	2:110:B:ALA:HB2	2:118:B:PRO:HA	10	0.48
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	2	0.48
(2,2628)	2:101:B:MET:HE3	2:103:B:TYR:HA	6	0.48
(2,2496)	1:51:A:LEU:HB2	1:51:A:LEU:HD12	5	0.48
(2,2450)	1:46:A:LEU:HB2	1:49:A:LYS:HE3	7	0.48
(2,2131)	1:17:A:HIS:HB3	1:14:A:LEU:HD11	10	0.48
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1992)	2:161:B:LYS:HE2	2:161:B:LYS:HD3	9	0.48
(2,1940)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.48
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	5	0.48
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	5	0.48
(2,1559)	1:56:A:ILE:HA	1:56:A:ILE:HG21	7	0.48
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	3	0.48
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD11	2	0.48
(2,1341)	1:15:A:ILE:HD11	1:15:A:ILE:HB	5	0.48
(2,1341)	1:15:A:ILE:HD11	1:15:A:ILE:HB	7	0.48
(2,1341)	1:15:A:ILE:HD11	1:15:A:ILE:HB	8	0.48
(2,1266)	1:1:A:MET:HG3	2:152:B:GLU:HG3	7	0.48
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	2	0.48
(2,1028)	2:134:B:ALA:HB1	2:124:B:LYS:HA	4	0.48
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	1	0.48
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	2	0.48
(2,920)	2:122:B:ASP:HA	2:125:B:LYS:HG3	5	0.48
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.48
(2,888)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.48
(2,846)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	5	0.48
(2,774)	2:101:B:MET:HE3	2:103:B:TYR:HA	6	0.48
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	2	0.48
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	5	0.48
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	8	0.48
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	1	0.48
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	3	0.48
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	4	0.48
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	10	0.48
(2,430)	1:15:A:ILE:HG22	2:106:B:SER:HA	4	0.48
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	2	0.48
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	5	0.48
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	2	0.48
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	3	0.48
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD23	2	0.48
(2,149)	1:58:A:SER:H	1:59:A:LEU:HD23	9	0.48
(2,31)	1:12:A:SER:H	2:109:B:LEU:HD12	8	0.48
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	2	0.48
(2,4562)	2:163:B:ALA:HA	2:163:B:ALA:H	9	0.47
(2,4521)	2:145:B:GLU:HG2	2:145:B:GLU:H	3	0.47
(2,4521)	2:145:B:GLU:HG2	2:145:B:GLU:H	7	0.47
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	2	0.47
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	6	0.47
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	1	0.47
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	2	0.47
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	3	0.47
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	4	0.47
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	8	0.47
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	10	0.47
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	5	0.47
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	2	0.47
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	4	0.47
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	7	0.47
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	8	0.47
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.47
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	1	0.47
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	9	0.47
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	4	0.47
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	5	0.47
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	10	0.47
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	5	0.47
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG23	3	0.47
(2,3416)	2:101:B:MET:HE2	1:17:A:HIS:HD2	4	0.47
(2,3307)	1:4:A:VAL:HG23	2:112:B:LEU:HA	1	0.47
(2,3296)	1:1:A:MET:HE2	2:156:B:ALA:HA	9	0.47
(2,3179)	2:154:B:VAL:HG13	2:155:B:ILE:H	1	0.47
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	5	0.47
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	7	0.47
(2,2888)	1:34:A:ALA:HB1	2:126:B:ILE:HD12	10	0.47
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	5	0.47
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	9	0.47
(2,2746)	2:112:B:LEU:HD23	1:7:A:LEU:HG	9	0.47
(2,2713)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.47
(2,2703)	2:109:B:LEU:HD12	2:109:B:LEU:H	3	0.47
(2,2691)	2:108:B:LEU:HD22	2:104:B:VAL:HB	3	0.47
(2,2588)	1:63:A:VAL:H	1:62:A:ASN:HB2	3	0.47
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	2	0.47
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	5	0.47
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	8	0.47
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	3	0.47
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	6	0.47
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	9	0.47
(2,2147)	1:15:A:ILE:HD13	2:103:B:TYR:HA	10	0.47
(2,2100)	1:10:A:ILE:HG23	1:47:A:PHE:HE2	9	0.47
(2,2072)	1:7:A:LEU:HD12	1:7:A:LEU:H	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1994)	2:161:B:LYS:HE3	2:161:B:LYS:HB2	4	0.47
(2,1949)	2:154:B:VAL:HG12	2:154:B:VAL:HA	9	0.47
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	2	0.47
(2,1848)	2:139:B:LEU:HA	2:139:B:LEU:HD13	4	0.47
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD2	9	0.47
(2,1742)	2:134:B:ALA:HB3	2:124:B:LYS:HA	8	0.47
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	5	0.47
(2,1491)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	6	0.47
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB3	2	0.47
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	5	0.47
(2,1283)	1:4:A:VAL:HG22	1:7:A:LEU:HD21	8	0.47
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD21	3	0.47
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD13	2	0.47
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB2	7	0.47
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	5	0.47
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG3	9	0.47
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	7	0.47
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	5	0.47
(2,907)	2:118:B:PRO:HG3	2:117:B:SER:HA	10	0.47
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	6	0.47
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	4	0.47
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	10	0.47
(2,609)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	2	0.47
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG22	5	0.47
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG23	8	0.47
(2,430)	1:15:A:ILE:HG22	2:106:B:SER:HA	2	0.47
(2,430)	1:15:A:ILE:HG23	2:106:B:SER:HA	7	0.47
(2,357)	1:4:A:VAL:HG22	2:112:B:LEU:HA	7	0.47
(2,317)	2:154:B:VAL:H	2:154:B:VAL:HG23	10	0.47
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD12	3	0.47
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD12	4	0.47
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD12	9	0.47
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD11	6	0.47
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD11	9	0.47
(2,217)	2:117:B:SER:H	2:115:B:ASN:HD21	2	0.47
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB3	6	0.47
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB1	4	0.47
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	5	0.47
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD11	5	0.47
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	10	0.46
(2,4410)	1:11:A:TYR:HA	1:11:A:TYR:HD2	3	0.46
(2,4376)	1:59:A:LEU:HB3	1:59:A:LEU:H	6	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	9	0.46
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	2	0.46
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	5	0.46
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	8	0.46
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	10	0.46
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	3	0.46
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	7	0.46
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	3	0.46
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	6	0.46
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	8	0.46
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	5	0.46
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	8	0.46
(2,3396)	1:39:A:VAL:HG21	2:109:B:LEU:HD13	1	0.46
(2,3305)	1:4:A:VAL:HG23	2:112:B:LEU:HA	2	0.46
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	5	0.46
(2,3172)	2:154:B:VAL:HG13	2:155:B:ILE:H	2	0.46
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	2	0.46
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	10	0.46
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	2	0.46
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	4	0.46
(2,3005)	2:138:B:ARG:HD2	2:135:B:ASP:H	4	0.46
(2,2897)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	10	0.46
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	8	0.46
(2,2851)	2:123:B:ILE:HG22	2:126:B:ILE:H	5	0.46
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	2	0.46
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	4	0.46
(2,2746)	2:112:B:LEU:HD22	1:7:A:LEU:HG	4	0.46
(2,2722)	2:110:B:ALA:HB1	2:109:B:LEU:HB3	10	0.46
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	4	0.46
(2,2346)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	6	0.46
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	10	0.46
(2,2204)	1:20:A:GLU:HG3	1:19:A:ASP:H	8	0.46
(2,2166)	1:16:A:LEU:HD12	1:27:A:LYS:HE3	8	0.46
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	4	0.46
(2,2030)	2:167:B:ALA:HB3	2:167:B:ALA:HA	2	0.46
(2,2030)	2:167:B:ALA:HB2	2:167:B:ALA:HA	3	0.46
(2,2030)	2:167:B:ALA:HB3	2:167:B:ALA:HA	4	0.46
(2,2030)	2:167:B:ALA:HB1	2:167:B:ALA:HA	5	0.46
(2,2030)	2:167:B:ALA:HB1	2:167:B:ALA:HA	9	0.46
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG12	2	0.46
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	4	0.46
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	2	0.46
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	4	0.46
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD2	10	0.46
(2,1659)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	10	0.46
(2,1614)	2:101:B:MET:HE2	1:14:A:LEU:HB2	1	0.46
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	2	0.46
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	5	0.46
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	8	0.46
(2,1491)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	4	0.46
(2,1391)	1:24:A:THR:HG23	1:27:A:LYS:HE3	9	0.46
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	4	0.46
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	5	0.46
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	7	0.46
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	5	0.46
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	4	0.46
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	5	0.46
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	9	0.46
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	2	0.46
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	4	0.46
(2,969)	2:127:B:LEU:HB2	2:124:B:LYS:HD2	10	0.46
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	2	0.46
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD12	4	0.46
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.46
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.46
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.46
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.46
(2,850)	2:110:B:ALA:HB2	2:118:B:PRO:HA	3	0.46
(2,567)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	6	0.46
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	10	0.46
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	2	0.46
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	10	0.46
(2,337)	2:169:B:GLY:H	2:168:B:GLY:HA3	4	0.46
(2,332)	2:165:B:VAL:H	2:164:B:SER:HB2	2	0.46
(2,329)	2:164:B:SER:H	2:162:B:LEU:HB3	7	0.46
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	7	0.46
(2,317)	2:154:B:VAL:H	2:154:B:VAL:HG23	4	0.46
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	9	0.46
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD11	10	0.46
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD12	1	0.46
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	8	0.46
(2,202)	2:114:B:GLY:H	2:115:B:ASN:HB3	3	0.46
(2,158)	1:63:A:VAL:H	1:63:A:VAL:HG13	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD11	3	0.46
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD11	10	0.46
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD13	10	0.46
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	9	0.46
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	2	0.45
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	6	0.45
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	3	0.45
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	4	0.45
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	7	0.45
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	9	0.45
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	3	0.45
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	2	0.45
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	9	0.45
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	1	0.45
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	2	0.45
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	8	0.45
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG21	6	0.45
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG21	8	0.45
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	4	0.45
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD23	5	0.45
(2,3385)	1:37:A:VAL:HG22	2:113:B:GLY:HA2	1	0.45
(2,3336)	1:15:A:ILE:HD11	2:109:B:LEU:HD23	6	0.45
(2,3305)	1:4:A:VAL:HG23	2:112:B:LEU:HA	8	0.45
(2,3300)	1:2:A:ALA:HB3	2:152:B:GLU:HG3	1	0.45
(2,3172)	2:154:B:VAL:HG12	2:155:B:ILE:H	5	0.45
(2,3172)	2:154:B:VAL:HG12	2:155:B:ILE:H	7	0.45
(2,3151)	2:152:B:GLU:HB2	2:151:B:ILE:HG22	1	0.45
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	2	0.45
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	7	0.45
(2,3123)	2:147:B:ASN:HB3	2:148:B:GLY:H	5	0.45
(2,3062)	2:142:B:VAL:HG21	2:104:B:VAL:HA	6	0.45
(2,3029)	2:139:B:LEU:HD22	2:124:B:LYS:HA	3	0.45
(2,3025)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	1	0.45
(2,3025)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	9	0.45
(2,2826)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	7	0.45
(2,2826)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	10	0.45
(2,2746)	2:112:B:LEU:HD22	1:7:A:LEU:HG	5	0.45
(2,2722)	2:110:B:ALA:HB3	2:109:B:LEU:HB3	6	0.45
(2,2716)	2:110:B:ALA:HB2	2:118:B:PRO:HA	3	0.45
(2,2703)	2:109:B:LEU:HD13	2:109:B:LEU:H	5	0.45
(2,2703)	2:109:B:LEU:HD13	2:109:B:LEU:H	6	0.45
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD13	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2456)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	4	0.45
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	5	0.45
(2,2147)	1:15:A:ILE:HD13	2:103:B:TYR:HA	8	0.45
(2,2094)	1:10:A:ILE:HD11	1:7:A:LEU:H	2	0.45
(2,2094)	1:10:A:ILE:HD11	1:7:A:LEU:H	7	0.45
(2,2030)	2:167:B:ALA:HB1	2:167:B:ALA:HA	1	0.45
(2,2030)	2:167:B:ALA:HB3	2:167:B:ALA:HA	6	0.45
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	4	0.45
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	9	0.45
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	1	0.45
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	2	0.45
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	5	0.45
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	9	0.45
(2,1659)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	8	0.45
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG3	3	0.45
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG11	2	0.45
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG11	3	0.45
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG11	7	0.45
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	5	0.45
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	4	0.45
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD12	10	0.45
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	4	0.45
(2,1341)	1:15:A:ILE:HD11	1:15:A:ILE:HB	10	0.45
(2,1283)	1:4:A:VAL:HG22	1:7:A:LEU:HD21	6	0.45
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB2	9	0.45
(2,1102)	2:143:B:ILE:HD12	2:107:B:TYR:HD2	10	0.45
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.45
(2,850)	2:110:B:ALA:HB2	2:118:B:PRO:HA	1	0.45
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	1	0.45
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	7	0.45
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	1	0.45
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	6	0.45
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	9	0.45
(2,621)	1:40:A:GLU:HG3	1:42:A:PHE:HE1	6	0.45
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	5	0.45
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	4	0.45
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	8	0.45
(2,439)	1:16:A:LEU:HD21	1:13:A:ALA:HA	10	0.45
(2,430)	1:15:A:ILE:HG22	2:106:B:SER:HA	9	0.45
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB2	8	0.45
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB2	4	0.45
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD13	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB2	3	0.45
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	4	0.45
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	6	0.45
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB3	8	0.45
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	4	0.45
(2,28)	1:11:A:TYR:H	1:9:A:CYS:HB3	6	0.45
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	8	0.44
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	1	0.44
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	6	0.44
(2,4197)	2:151:B:ILE:HA	2:151:B:ILE:HG12	9	0.44
(2,4067)	1:11:A:TYR:HA	1:11:A:TYR:HD2	3	0.44
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	3	0.44
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	10	0.44
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD13	9	0.44
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG22	4	0.44
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG21	7	0.44
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG23	9	0.44
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	6	0.44
(2,3495)	2:156:B:ALA:HB1	1:7:A:LEU:HD13	4	0.44
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD21	2	0.44
(2,3373)	1:34:A:ALA:HB1	2:125:B:LYS:HE2	5	0.44
(2,3297)	1:1:A:MET:HE3	2:152:B:GLU:HA	3	0.44
(2,3062)	2:142:B:VAL:HG21	2:104:B:VAL:HA	3	0.44
(2,3054)	2:142:B:VAL:HG13	2:107:B:TYR:HD2	4	0.44
(2,3025)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	7	0.44
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	2	0.44
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE2	6	0.44
(2,2826)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	8	0.44
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.44
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.44
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.44
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	1	0.44
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	10	0.44
(2,2722)	2:110:B:ALA:HB3	2:109:B:LEU:HB3	5	0.44
(2,2716)	2:110:B:ALA:HB2	2:118:B:PRO:HA	1	0.44
(2,2714)	2:110:B:ALA:HB1	2:123:B:ILE:H	9	0.44
(2,2703)	2:109:B:LEU:HD12	2:109:B:LEU:H	8	0.44
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	7	0.44
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	8	0.44
(2,2681)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	9	0.44
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	1	0.44
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	9	0.44
(2,2456)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	6	0.44
(2,2410)	1:40:A:GLU:HG3	1:42:A:PHE:HE1	6	0.44
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	1	0.44
(2,2341)	1:34:A:ALA:HB1	2:125:B:LYS:HE2	5	0.44
(2,2328)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	4	0.44
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	2	0.44
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	4	0.44
(2,2094)	1:10:A:ILE:HD13	1:7:A:LEU:H	6	0.44
(2,2072)	1:7:A:LEU:HD11	1:7:A:LEU:H	8	0.44
(2,2030)	2:167:B:ALA:HB2	2:167:B:ALA:HA	7	0.44
(2,2004)	2:163:B:ALA:HB2	2:163:B:ALA:HA	9	0.44
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	5	0.44
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD3	4	0.44
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	2	0.44
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	3	0.44
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	8	0.44
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	4	0.44
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	6	0.44
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG11	1	0.44
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG12	8	0.44
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG12	9	0.44
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD13	3	0.44
(2,1391)	1:24:A:THR:HG21	1:27:A:LYS:HE3	8	0.44
(2,1341)	1:15:A:ILE:HD13	1:15:A:ILE:HB	2	0.44
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	3	0.44
(2,1255)	2:165:B:VAL:HG11	2:166:B:PRO:HD2	7	0.44
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB2	5	0.44
(2,1054)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	10	0.44
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD12	7	0.44
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.44
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.44
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.44
(2,761)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	0.44
(2,628)	1:40:A:GLU:HG3	1:41:A:PRO:HD3	8	0.44
(2,569)	1:34:A:ALA:HB1	2:125:B:LYS:HE2	5	0.44
(2,558)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	9	0.44
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	2	0.44
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	4	0.44
(2,471)	1:22:A:THR:HB	1:22:A:THR:HG22	9	0.44
(2,430)	1:15:A:ILE:HG22	2:106:B:SER:HA	1	0.44
(2,430)	1:15:A:ILE:HG23	2:106:B:SER:HA	10	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:10:A:ILE:HG22	2:159:B:ILE:HG12	1	0.44
(2,391)	1:10:A:ILE:HG22	2:159:B:ILE:HG12	9	0.44
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	2	0.44
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE2	6	0.44
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD12	2	0.44
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	4	0.44
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD13	9	0.44
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	1	0.44
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	3	0.43
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	3	0.43
(2,4206)	2:159:B:ILE:HA	2:159:B:ILE:HG12	5	0.43
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD13	8	0.43
(2,4141)	1:27:A:LYS:HA	1:27:A:LYS:HD2	9	0.43
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	4	0.43
(2,3858)	2:125:B:LYS:H	2:125:B:LYS:HB2	5	0.43
(2,3841)	2:122:B:ASP:H	2:122:B:ASP:HB3	6	0.43
(2,3495)	2:156:B:ALA:HB1	1:7:A:LEU:HD13	6	0.43
(2,3416)	2:101:B:MET:HE1	1:17:A:HIS:HD2	8	0.43
(2,3416)	2:101:B:MET:HE2	1:17:A:HIS:HD2	9	0.43
(2,3296)	1:1:A:MET:HE1	2:156:B:ALA:HA	2	0.43
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	5	0.43
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	1	0.43
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	3	0.43
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	4	0.43
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD13	8	0.43
(2,3029)	2:139:B:LEU:HD22	2:124:B:LYS:HA	2	0.43
(2,2965)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	5	0.43
(2,2959)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	5	0.43
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	4	0.43
(2,2826)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	3	0.43
(2,2826)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	5	0.43
(2,2822)	2:120:B:ALA:HB3	2:140:B:ASN:H	3	0.43
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.43
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.43
(2,2768)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.43
(2,2703)	2:109:B:LEU:HD12	2:109:B:LEU:H	1	0.43
(2,2588)	1:63:A:VAL:H	1:62:A:ASN:HB2	1	0.43
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	5	0.43
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	5	0.43
(2,2251)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	2	0.43
(2,2147)	1:15:A:ILE:HD11	2:103:B:TYR:HA	3	0.43
(2,2071)	1:7:A:LEU:HD23	1:11:A:TYR:HE1	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2030)	2:167:B:ALA:HB2	2:167:B:ALA:HA	10	0.43
(2,1898)	2:146:B:LEU:HD12	2:151:B:ILE:HG13	3	0.43
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	6	0.43
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	8	0.43
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	10	0.43
(2,1614)	2:101:B:MET:HE2	1:14:A:LEU:HB2	7	0.43
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG13	4	0.43
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG11	6	0.43
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	4	0.43
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	9	0.43
(2,1542)	1:51:A:LEU:HD21	1:56:A:ILE:HB	8	0.43
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	1	0.43
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	6	0.43
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	9	0.43
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD11	7	0.43
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB3	2	0.43
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	5	0.43
(2,1341)	1:15:A:ILE:HD13	1:15:A:ILE:HB	9	0.43
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG22	9	0.43
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	9	0.43
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD12	9	0.43
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD13	8	0.43
(2,1102)	2:143:B:ILE:HD13	2:107:B:TYR:HD2	4	0.43
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD13	8	0.43
(2,1017)	2:132:B:ILE:HG23	2:133:B:GLU:HB3	5	0.43
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	2	0.43
(2,728)	1:54:A:VAL:HG22	1:58:A:SER:HB2	8	0.43
(2,587)	1:37:A:VAL:HG22	2:112:B:LEU:HD23	2	0.43
(2,558)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	10	0.43
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	3	0.43
(2,430)	1:15:A:ILE:HG23	2:106:B:SER:HA	6	0.43
(2,334)	2:167:B:ALA:H	2:167:B:ALA:HB3	8	0.43
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	3	0.43
(2,317)	2:154:B:VAL:H	2:154:B:VAL:HG23	2	0.43
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	4	0.43
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD13	5	0.43
(2,225)	2:120:B:ALA:H	2:143:B:ILE:HD11	7	0.43
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB3	7	0.43
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG11	1	0.43
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	3	0.43
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB2	4	0.43
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	1	0.43
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	2	0.43
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	3	0.43
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	5	0.43
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	7	0.43
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	8	0.43
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	9	0.43
(2,170)	1:43:A:TRP:HE1	1:43:A:TRP:HB2	10	0.43
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD23	2	0.43
(2,73)	1:27:A:LYS:H	2:130:B:VAL:HG11	9	0.43
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD12	2	0.43
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD12	5	0.43
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	7	0.42
(2,4172)	2:105:B:ALA:HA	2:108:B:LEU:HB3	8	0.42
(2,4118)	2:155:B:ILE:HA	2:155:B:ILE:HG12	1	0.42
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	1	0.42
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	2	0.42
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	5	0.42
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	8	0.42
(2,4069)	2:105:B:ALA:HA	2:108:B:LEU:HB3	8	0.42
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	7	0.42
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG23	5	0.42
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	6	0.42
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD21	3	0.42
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD21	7	0.42
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	4	0.42
(2,3305)	1:4:A:VAL:HG11	2:112:B:LEU:HA	6	0.42
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	2	0.42
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	8	0.42
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB2	1	0.42
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB2	10	0.42
(2,3055)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.42
(2,3055)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.42
(2,3050)	2:142:B:VAL:HA	2:142:B:VAL:HG21	9	0.42
(2,3025)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	8	0.42
(2,2991)	2:137:B:ASP:HA	2:141:B:LYS:HB2	9	0.42
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	10	0.42
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.42
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.42
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.42
(2,2715)	2:110:B:ALA:HB2	2:115:B:ASN:H	7	0.42
(2,2714)	2:110:B:ALA:HB3	2:123:B:ILE:H	2	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2612)	1:42:A:PHE:HD1	1:42:A:PHE:HZ	1	0.42
(2,2612)	1:42:A:PHE:HD1	1:42:A:PHE:HZ	2	0.42
(2,2612)	1:42:A:PHE:HD1	1:42:A:PHE:HZ	3	0.42
(2,2612)	1:42:A:PHE:HD2	1:42:A:PHE:HZ	5	0.42
(2,2612)	1:42:A:PHE:HD1	1:42:A:PHE:HZ	7	0.42
(2,2612)	1:42:A:PHE:HD1	1:42:A:PHE:HZ	8	0.42
(2,2612)	1:42:A:PHE:HD1	1:42:A:PHE:HZ	9	0.42
(2,2612)	1:42:A:PHE:HD2	1:42:A:PHE:HZ	10	0.42
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	2	0.42
(2,2581)	1:61:A:CYS:HB2	1:60:A:ILE:H	10	0.42
(2,2480)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	7	0.42
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG23	6	0.42
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	9	0.42
(2,2204)	1:20:A:GLU:HG3	1:19:A:ASP:H	5	0.42
(2,2204)	1:20:A:GLU:HG3	1:19:A:ASP:H	7	0.42
(2,2147)	1:15:A:ILE:HD11	2:103:B:TYR:HA	6	0.42
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE1	6	0.42
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	10	0.42
(2,2094)	1:10:A:ILE:HD11	1:7:A:LEU:H	10	0.42
(2,2034)	1:2:A:ALA:HB2	1:6:A:GLU:H	7	0.42
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB2	4	0.42
(2,2004)	2:163:B:ALA:HB1	2:163:B:ALA:HA	8	0.42
(2,1992)	2:161:B:LYS:HE3	2:161:B:LYS:HD2	5	0.42
(2,1992)	2:161:B:LYS:HE3	2:161:B:LYS:HD2	6	0.42
(2,1992)	2:161:B:LYS:HE2	2:161:B:LYS:HD3	10	0.42
(2,1948)	2:154:B:VAL:HG22	2:149:B:LYS:HD2	8	0.42
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	8	0.42
(2,1829)	2:137:B:ASP:HA	2:141:B:LYS:HB2	9	0.42
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	6	0.42
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	9	0.42
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	1	0.42
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	8	0.42
(2,1659)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	5	0.42
(2,1659)	2:111:B:ALA:HB2	2:151:B:ILE:HD12	7	0.42
(2,1613)	2:101:B:MET:HE3	2:101:B:MET:HG2	1	0.42
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG13	10	0.42
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	8	0.42
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	3	0.42
(2,1283)	1:4:A:VAL:HG23	1:7:A:LEU:HD21	5	0.42
(2,1283)	1:4:A:VAL:HG21	1:7:A:LEU:HD21	7	0.42
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB3	2	0.42
(2,1054)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1054)	2:139:B:LEU:HD23	2:124:B:LYS:HE2	9	0.42
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD12	8	0.42
(2,1041)	2:137:B:ASP:HA	2:141:B:LYS:HB2	9	0.42
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.42
(2,885)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.42
(2,866)	2:112:B:LEU:HD12	2:108:B:LEU:HB2	3	0.42
(2,800)	2:105:B:ALA:HB3	2:101:B:MET:HG2	1	0.42
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	6	0.42
(2,707)	1:54:A:VAL:HG22	1:58:A:SER:HB2	8	0.42
(2,679)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	7	0.42
(2,609)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	9	0.42
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	2	0.42
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG12	2	0.42
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB2	1	0.42
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	10	0.42
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB3	4	0.42
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB3	9	0.42
(2,202)	2:114:B:GLY:H	2:115:B:ASN:HB3	1	0.42
(2,189)	2:112:B:LEU:H	2:112:B:LEU:HD12	1	0.42
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	7	0.42
(2,179)	2:107:B:TYR:H	2:107:B:TYR:HD2	8	0.42
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG23	10	0.42
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG11	7	0.42
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG13	10	0.42
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB2	1	0.42
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	7	0.41
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	4	0.41
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	4	0.41
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	7	0.41
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	10	0.41
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD21	8	0.41
(2,3402)	1:59:A:LEU:HD11	2:159:B:ILE:HA	1	0.41
(2,3399)	1:59:A:LEU:HD11	2:159:B:ILE:HA	1	0.41
(2,3355)	1:21:A:VAL:HG13	2:132:B:ILE:HB	10	0.41
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	4	0.41
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	9	0.41
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	9	0.41
(2,3123)	2:147:B:ASN:HB2	2:148:B:GLY:H	6	0.41
(2,3120)	2:147:B:ASN:HB2	2:148:B:GLY:H	9	0.41
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB2	6	0.41
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	9	0.41
(2,3055)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	8	0.41
(2,2950)	2:132:B:ILE:HD11	2:130:B:VAL:H	5	0.41
(2,2916)	2:128:B:ASP:HB2	2:124:B:LYS:HB3	3	0.41
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	3	0.41
(2,2850)	2:123:B:ILE:HG23	2:139:B:LEU:HA	9	0.41
(2,2849)	2:123:B:ILE:HG21	2:106:B:SER:HA	4	0.41
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	9	0.41
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	7	0.41
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	6	0.41
(2,2647)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	5	0.41
(2,2612)	1:42:A:PHE:HD2	1:42:A:PHE:HZ	4	0.41
(2,2612)	1:42:A:PHE:HD2	1:42:A:PHE:HZ	6	0.41
(2,2388)	1:38:A:ASN:HB2	1:39:A:VAL:HG22	8	0.41
(2,2260)	1:25:A:GLU:HG2	1:25:A:GLU:H	7	0.41
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	3	0.41
(2,2030)	2:167:B:ALA:HB1	2:167:B:ALA:HA	8	0.41
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	6	0.41
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG12	6	0.41
(2,1864)	2:142:B:VAL:HA	2:142:B:VAL:HG21	9	0.41
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD2	6	0.41
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	1	0.41
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	10	0.41
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	6	0.41
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	9	0.41
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	7	0.41
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	1	0.41
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	6	0.41
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	7	0.41
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	8	0.41
(2,1542)	1:51:A:LEU:HD22	1:56:A:ILE:HB	1	0.41
(2,1529)	1:49:A:LYS:HD3	1:49:A:LYS:HG2	7	0.41
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	4	0.41
(2,1341)	1:15:A:ILE:HD13	1:15:A:ILE:HB	1	0.41
(2,1283)	1:4:A:VAL:HG22	1:7:A:LEU:HD21	9	0.41
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB1	3	0.41
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB3	6	0.41
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	9	0.41
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD12	5	0.41
(2,1102)	2:143:B:ILE:HD13	2:107:B:TYR:HD2	3	0.41
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	9	0.41
(2,1054)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	7	0.41
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD12	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG2	2	0.41
(2,937)	2:123:B:ILE:HG21	2:106:B:SER:HA	4	0.41
(2,919)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	6	0.41
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD11	9	0.41
(2,847)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	4	0.41
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	8	0.41
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	9	0.41
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	3	0.41
(2,426)	1:15:A:ILE:HG21	1:18:A:ASP:HB3	10	0.41
(2,414)	1:14:A:LEU:HD12	2:101:B:MET:HG3	8	0.41
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	9	0.41
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	9	0.41
(2,329)	2:164:B:SER:H	2:162:B:LEU:HB3	10	0.41
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	10	0.41
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	10	0.41
(2,294)	2:144:B:SER:H	2:143:B:ILE:HD11	1	0.41
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB2	2	0.41
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD2	1	0.41
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	3	0.41
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	9	0.41
(2,136)	1:51:A:LEU:H	1:50:A:ALA:HB2	1	0.41
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD13	4	0.41
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	5	0.41
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG11	8	0.41
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB1	6	0.41
(2,4375)	1:59:A:LEU:HB3	1:60:A:ILE:HB	8	0.4
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.4
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	1	0.4
(2,4117)	2:155:B:ILE:HA	2:155:B:ILE:HG12	1	0.4
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	3	0.4
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	6	0.4
(2,4110)	2:151:B:ILE:HA	2:151:B:ILE:HG12	9	0.4
(2,4049)	1:59:A:LEU:HB3	1:60:A:ILE:HB	8	0.4
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	4	0.4
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG23	1	0.4
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG21	10	0.4
(2,3492)	2:152:B:GLU:HG2	1:7:A:LEU:HB3	1	0.4
(2,3464)	2:129:B:SER:HA	1:30:A:ALA:HA	8	0.4
(2,3361)	1:31:A:LEU:HD13	2:129:B:SER:HA	8	0.4
(2,3355)	1:21:A:VAL:HG13	2:132:B:ILE:HB	4	0.4
(2,3301)	1:2:A:ALA:HB3	2:152:B:GLU:HA	4	0.4
(2,3298)	1:1:A:MET:HG3	2:153:B:ASP:HB3	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3297)	1:1:A:MET:HE3	2:152:B:GLU:HA	5	0.4
(2,3296)	1:1:A:MET:HE3	2:156:B:ALA:HA	5	0.4
(2,3270)	2:165:B:VAL:HG13	2:161:B:LYS:HG3	7	0.4
(2,3172)	2:154:B:VAL:HG13	2:155:B:ILE:H	4	0.4
(2,3172)	2:154:B:VAL:HG11	2:155:B:ILE:H	6	0.4
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	5	0.4
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	6	0.4
(2,3120)	2:147:B:ASN:HB2	2:148:B:GLY:H	2	0.4
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.4
(2,3054)	2:142:B:VAL:HG11	2:107:B:TYR:HD2	10	0.4
(2,2982)	2:134:B:ALA:HB3	2:124:B:LYS:HA	3	0.4
(2,2858)	2:124:B:LYS:H	2:124:B:LYS:HE3	1	0.4
(2,2842)	2:123:B:ILE:HG21	2:139:B:LEU:H	2	0.4
(2,2808)	2:119:B:SER:HB2	2:121:B:LYS:HD3	6	0.4
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.4
(2,2800)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.4
(2,2722)	2:110:B:ALA:HB3	2:109:B:LEU:HB3	2	0.4
(2,2715)	2:110:B:ALA:HB1	2:115:B:ASN:H	2	0.4
(2,2703)	2:109:B:LEU:HD12	2:109:B:LEU:H	10	0.4
(2,2639)	2:104:B:VAL:HA	2:146:B:LEU:HD23	1	0.4
(2,2579)	1:61:A:CYS:HB3	1:62:A:ASN:HD21	1	0.4
(2,2561)	1:59:A:LEU:HD13	1:56:A:ILE:HA	6	0.4
(2,2557)	1:59:A:LEU:HD13	1:56:A:ILE:HA	6	0.4
(2,2456)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	2	0.4
(2,2456)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	8	0.4
(2,2410)	1:40:A:GLU:HG3	1:42:A:PHE:HE1	4	0.4
(2,2388)	1:37:A:VAL:HG23	1:38:A:ASN:HB3	2	0.4
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	4	0.4
(2,2250)	1:25:A:GLU:HB3	1:28:A:ILE:H	4	0.4
(2,2162)	1:16:A:LEU:HD21	1:13:A:ALA:HA	10	0.4
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	5	0.4
(2,2147)	1:15:A:ILE:HD11	2:103:B:TYR:HA	5	0.4
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	3	0.4
(2,2004)	2:163:B:ALA:HB1	2:163:B:ALA:HA	3	0.4
(2,2004)	2:163:B:ALA:HB1	2:163:B:ALA:HA	7	0.4
(2,1992)	2:161:B:LYS:HE2	2:161:B:LYS:HD3	4	0.4
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD2	8	0.4
(2,1715)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	6	0.4
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	3	0.4
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	2	0.4
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	3	0.4
(2,1701)	2:120:B:ALA:HB2	2:139:B:LEU:HB2	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1701)	2:120:B:ALA:HB3	2:139:B:LEU:HB2	6	0.4
(2,1686)	2:118:B:PRO:HA	2:118:B:PRO:HD3	3	0.4
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB3	9	0.4
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	1	0.4
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG3	7	0.4
(2,1609)	1:63:A:VAL:HB	1:63:A:VAL:HG22	5	0.4
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	2	0.4
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	2	0.4
(2,1354)	1:16:A:LEU:HD11	1:27:A:LYS:HD3	6	0.4
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG23	6	0.4
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG22	8	0.4
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	1	0.4
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.4
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	5	0.4
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	10	0.4
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.4
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD11	6	0.4
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD13	5	0.4
(2,919)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	2	0.4
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	4	0.4
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	3	0.4
(2,739)	1:59:A:LEU:HD12	1:56:A:ILE:HA	2	0.4
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG21	6	0.4
(2,621)	1:40:A:GLU:HG3	1:42:A:PHE:HE1	4	0.4
(2,492)	1:25:A:GLU:HA	1:25:A:GLU:HG2	5	0.4
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	4	0.4
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	7	0.4
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	3	0.4
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	3	0.4
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD11	5	0.4
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD13	10	0.4
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB2	10	0.4
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD23	8	0.4
(2,239)	2:124:B:LYS:H	2:124:B:LYS:HE3	1	0.4
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB3	5	0.4
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB2	6	0.4
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	5	0.4
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB2	2	0.4
(2,160)	1:64:A:GLY:H	1:63:A:VAL:HG23	5	0.4
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD13	7	0.4
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG21	5	0.4
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG23	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	7	0.39
(2,4549)	2:155:B:ILE:HD12	2:155:B:ILE:HB	9	0.39
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD12	2	0.39
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	8	0.39
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	6	0.39
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	8	0.39
(2,3492)	2:152:B:GLU:HG2	1:7:A:LEU:HB3	3	0.39
(2,3416)	2:101:B:MET:HE1	1:17:A:HIS:HD2	6	0.39
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	10	0.39
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	10	0.39
(2,3361)	1:31:A:LEU:HD13	2:129:B:SER:HA	4	0.39
(2,3355)	1:21:A:VAL:HG13	2:132:B:ILE:HB	1	0.39
(2,3331)	1:14:A:LEU:HD22	2:159:B:ILE:HA	5	0.39
(2,3296)	1:1:A:MET:HE1	2:156:B:ALA:HA	8	0.39
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG22	9	0.39
(2,3172)	2:154:B:VAL:HG13	2:155:B:ILE:H	10	0.39
(2,3140)	2:151:B:ILE:HD11	2:149:B:LYS:H	5	0.39
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB2	7	0.39
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD12	4	0.39
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD11	10	0.39
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD12	2	0.39
(2,3067)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	8	0.39
(2,3054)	2:142:B:VAL:HG12	2:107:B:TYR:HD2	6	0.39
(2,3049)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	7	0.39
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	9	0.39
(2,2921)	1:31:A:LEU:HD13	2:129:B:SER:HA	4	0.39
(2,2849)	2:123:B:ILE:HG21	2:106:B:SER:HA	3	0.39
(2,2849)	2:123:B:ILE:HG21	2:106:B:SER:HA	9	0.39
(2,2826)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	4	0.39
(2,2816)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	8	0.39
(2,2808)	2:119:B:SER:HB2	2:121:B:LYS:HD3	3	0.39
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	2	0.39
(2,2723)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.39
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	2	0.39
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB3	9	0.39
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	7	0.39
(2,2462)	1:47:A:PHE:HB2	1:51:A:LEU:HD11	1	0.39
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG22	3	0.39
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	10	0.39
(2,2339)	1:33:A:LYS:H	1:33:A:LYS:HG3	8	0.39
(2,2328)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	5	0.39
(2,2166)	1:16:A:LEU:HD23	1:27:A:LYS:HE3	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	6	0.39
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	8	0.39
(2,2094)	1:10:A:ILE:HD11	1:7:A:LEU:H	4	0.39
(2,2094)	1:10:A:ILE:HD11	1:7:A:LEU:H	5	0.39
(2,2094)	1:10:A:ILE:HD11	1:7:A:LEU:H	9	0.39
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB2	10	0.39
(2,1992)	2:161:B:LYS:HE2	2:161:B:LYS:HD3	7	0.39
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	10	0.39
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	1	0.39
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	5	0.39
(2,1703)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	8	0.39
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG2	2	0.39
(2,1629)	2:105:B:ALA:HB2	2:101:B:MET:HG3	8	0.39
(2,1614)	2:101:B:MET:HE2	1:14:A:LEU:HB2	9	0.39
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG11	1	0.39
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG11	4	0.39
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG12	6	0.39
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD11	8	0.39
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD12	2	0.39
(2,1099)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	8	0.39
(2,1081)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	7	0.39
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD12	2	0.39
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG3	4	0.39
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD13	1	0.39
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD11	3	0.39
(2,1028)	2:134:B:ALA:HB3	2:124:B:LYS:HA	3	0.39
(2,937)	2:123:B:ILE:HG21	2:106:B:SER:HA	3	0.39
(2,937)	2:123:B:ILE:HG21	2:106:B:SER:HA	9	0.39
(2,916)	2:120:B:ALA:HB2	2:143:B:ILE:HD13	8	0.39
(2,772)	2:101:B:MET:HE3	2:105:B:ALA:HB2	9	0.39
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG23	1	0.39
(2,587)	1:37:A:VAL:HG22	2:112:B:LEU:HD21	6	0.39
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	3	0.39
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	1	0.39
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	5	0.39
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	8	0.39
(2,430)	1:15:A:ILE:HG23	2:106:B:SER:HA	8	0.39
(2,325)	2:161:B:LYS:H	2:161:B:LYS:HB2	8	0.39
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	2	0.39
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	3	0.39
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	6	0.39
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD13	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD3	2	0.39
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB1	8	0.39
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB1	7	0.39
(2,70)	1:26:A:ASP:H	1:25:A:GLU:HB2	9	0.39
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	3	0.39
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD11	3	0.39
(2,4521)	2:145:B:GLU:HG2	2:145:B:GLU:H	10	0.38
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD11	9	0.38
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	9	0.38
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD21	6	0.38
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	7	0.38
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	7	0.38
(2,3355)	1:21:A:VAL:HG13	2:132:B:ILE:HB	2	0.38
(2,3342)	1:15:A:ILE:HD13	2:106:B:SER:HA	4	0.38
(2,3336)	1:15:A:ILE:HD11	2:109:B:LEU:HD23	8	0.38
(2,3331)	1:14:A:LEU:HD23	2:159:B:ILE:HA	7	0.38
(2,3270)	2:165:B:VAL:HG12	2:161:B:LYS:HG3	9	0.38
(2,3195)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	7	0.38
(2,3123)	2:147:B:ASN:HB3	2:148:B:GLY:H	8	0.38
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD11	9	0.38
(2,3025)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	3	0.38
(2,2715)	2:110:B:ALA:HB2	2:115:B:ASN:H	9	0.38
(2,2715)	2:110:B:ALA:HB2	2:115:B:ASN:H	10	0.38
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	9	0.38
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG13	10	0.38
(2,2456)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	1	0.38
(2,2456)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	5	0.38
(2,2456)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	7	0.38
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	9	0.38
(2,2337)	1:33:A:LYS:H	1:33:A:LYS:HG3	8	0.38
(2,2286)	1:28:A:ILE:HD12	1:44:A:PRO:HA	3	0.38
(2,2260)	1:25:A:GLU:HG2	1:25:A:GLU:H	4	0.38
(2,2204)	1:20:A:GLU:HG3	1:19:A:ASP:H	3	0.38
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD13	10	0.38
(2,2094)	1:10:A:ILE:HD13	1:7:A:LEU:H	3	0.38
(2,2004)	2:163:B:ALA:HB3	2:163:B:ALA:HA	1	0.38
(2,1992)	2:161:B:LYS:HE2	2:161:B:LYS:HD3	1	0.38
(2,1881)	2:144:B:SER:HA	2:147:B:ASN:HB2	3	0.38
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	4	0.38
(2,1742)	2:134:B:ALA:HB1	2:124:B:LYS:HA	4	0.38
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD3	6	0.38
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1700)	2:139:B:LEU:HD12	2:120:B:ALA:HA	6	0.38
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	2	0.38
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD13	4	0.38
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD12	9	0.38
(2,1510)	1:28:A:ILE:HD12	1:44:A:PRO:HA	3	0.38
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	6	0.38
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	3	0.38
(2,1283)	1:4:A:VAL:HG22	1:7:A:LEU:HD21	2	0.38
(2,1283)	1:4:A:VAL:HG21	1:7:A:LEU:HD21	3	0.38
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	5	0.38
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG22	9	0.38
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG12	2	0.38
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG13	3	0.38
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG11	9	0.38
(2,1173)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	1	0.38
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.38
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD11	9	0.38
(2,1090)	2:142:B:VAL:HG22	2:146:B:LEU:HD22	7	0.38
(2,1085)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.38
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD11	9	0.38
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	6	0.38
(2,1054)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	8	0.38
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD13	7	0.38
(2,919)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	9	0.38
(2,875)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.38
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	8	0.38
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	10	0.38
(2,683)	1:50:A:ALA:HB3	1:54:A:VAL:HG22	9	0.38
(2,657)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	4	0.38
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	1	0.38
(2,522)	1:28:A:ILE:HD12	1:44:A:PRO:HA	3	0.38
(2,430)	1:15:A:ILE:HG23	2:106:B:SER:HA	3	0.38
(2,430)	1:15:A:ILE:HG23	2:106:B:SER:HA	5	0.38
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE1	6	0.38
(2,357)	1:4:A:VAL:HG22	2:112:B:LEU:HA	3	0.38
(2,337)	2:169:B:GLY:H	2:168:B:GLY:HA3	10	0.38
(2,317)	2:154:B:VAL:H	2:154:B:VAL:HG23	9	0.38
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB3	7	0.38
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG12	7	0.38
(2,189)	2:112:B:LEU:H	2:112:B:LEU:HD12	3	0.38
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB2	6	0.38
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG21	7	0.38
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	9	0.38
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	10	0.37
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	2	0.37
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	5	0.37
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	6	0.37
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	10	0.37
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	9	0.37
(2,3506)	1:60:A:ILE:HB	2:159:B:ILE:HG23	2	0.37
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	10	0.37
(2,3460)	1:35:A:ALA:HB3	2:126:B:ILE:HG21	6	0.37
(2,3445)	2:112:B:LEU:HA	1:37:A:VAL:HG21	3	0.37
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	4	0.37
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	9	0.37
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	4	0.37
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	9	0.37
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	10	0.37
(2,3305)	1:4:A:VAL:HG11	2:112:B:LEU:HA	4	0.37
(2,3301)	1:2:A:ALA:HB3	2:152:B:GLU:HA	7	0.37
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG11	1	0.37
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.37
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	3	0.37
(2,3231)	2:159:B:ILE:HG21	2:159:B:ILE:H	7	0.37
(2,3205)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	3	0.37
(2,3123)	2:147:B:ASN:HB3	2:148:B:GLY:H	3	0.37
(2,3123)	2:147:B:ASN:HB2	2:148:B:GLY:H	10	0.37
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB2	9	0.37
(2,2982)	2:134:B:ALA:HB3	2:124:B:LYS:HA	6	0.37
(2,2916)	2:128:B:ASP:HB2	2:124:B:LYS:HB3	6	0.37
(2,2714)	2:110:B:ALA:HB1	2:123:B:ILE:H	3	0.37
(2,2706)	1:8:A:ALA:HA	2:109:B:LEU:HD13	5	0.37
(2,2703)	2:109:B:LEU:HD13	2:109:B:LEU:H	9	0.37
(2,2540)	1:54:A:VAL:HG22	1:58:A:SER:HB2	8	0.37
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD11	6	0.37
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	7	0.37
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	3	0.37
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	6	0.37
(2,2260)	1:25:A:GLU:HG2	1:25:A:GLU:H	1	0.37
(2,2160)	1:16:A:LEU:HD12	1:21:A:VAL:H	1	0.37
(2,2160)	1:16:A:LEU:HD11	1:21:A:VAL:H	10	0.37
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	1	0.37
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	10	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2100)	1:10:A:ILE:HG23	1:47:A:PHE:HE2	1	0.37
(2,2034)	1:2:A:ALA:HB2	1:6:A:GLU:H	3	0.37
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	7	0.37
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	9	0.37
(2,2004)	2:163:B:ALA:HB3	2:163:B:ALA:HA	4	0.37
(2,2004)	2:163:B:ALA:HB3	2:163:B:ALA:HA	5	0.37
(2,1989)	2:161:B:LYS:HA	2:161:B:LYS:HG2	9	0.37
(2,1946)	2:154:B:VAL:HG22	2:149:B:LYS:HG2	1	0.37
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.37
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	10	0.37
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	1	0.37
(2,1712)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	6	0.37
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	4	0.37
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	9	0.37
(2,1589)	1:60:A:ILE:HD12	1:60:A:ILE:HA	10	0.37
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	4	0.37
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	1	0.37
(2,1383)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	7	0.37
(2,1373)	1:22:A:THR:HG21	1:21:A:VAL:HB	6	0.37
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG13	5	0.37
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG11	8	0.37
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	9	0.37
(2,1219)	2:161:B:LYS:HA	2:161:B:LYS:HG2	9	0.37
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	3	0.37
(2,1186)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	7	0.37
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	5	0.37
(2,1122)	2:146:B:LEU:HA	2:146:B:LEU:HD11	7	0.37
(2,1085)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.37
(2,1085)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.37
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD11	4	0.37
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG2	10	0.37
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD11	2	0.37
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD13	9	0.37
(2,1028)	2:134:B:ALA:HB3	2:124:B:LYS:HA	6	0.37
(2,772)	2:101:B:MET:HE3	2:105:B:ALA:HB2	4	0.37
(2,739)	1:59:A:LEU:HD12	1:56:A:ILE:HA	1	0.37
(2,736)	1:59:A:LEU:HD22	1:59:A:LEU:HG	7	0.37
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG23	10	0.37
(2,657)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	6	0.37
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	2	0.37
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	7	0.37
(2,609)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,587)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	5	0.37
(2,587)	1:37:A:VAL:HG21	2:112:B:LEU:HD21	9	0.37
(2,587)	1:37:A:VAL:HG22	2:112:B:LEU:HD21	10	0.37
(2,493)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	3	0.37
(2,492)	1:25:A:GLU:HA	1:25:A:GLU:HG2	10	0.37
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	1	0.37
(2,422)	1:15:A:ILE:HD11	2:106:B:SER:HB2	8	0.37
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	5	0.37
(2,325)	2:161:B:LYS:H	2:161:B:LYS:HB2	2	0.37
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB3	6	0.37
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG12	8	0.37
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB2	8	0.37
(2,128)	1:48:A:ALA:H	1:28:A:ILE:HD12	1	0.37
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG23	8	0.37
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG21	9	0.37
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB3	4	0.37
(2,44)	1:16:A:LEU:H	1:13:A:ALA:HB3	9	0.37
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	3	0.36
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	7	0.36
(2,4120)	2:155:B:ILE:HD12	2:155:B:ILE:HB	9	0.36
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	1	0.36
(2,3460)	1:35:A:ALA:HB1	2:126:B:ILE:HG22	4	0.36
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	7	0.36
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	6	0.36
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	6	0.36
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	8	0.36
(2,3355)	1:21:A:VAL:HG11	2:132:B:ILE:HB	8	0.36
(2,3307)	1:4:A:VAL:HG23	2:112:B:LEU:HA	9	0.36
(2,3301)	1:2:A:ALA:HB3	2:152:B:GLU:HA	5	0.36
(2,3301)	1:2:A:ALA:HB3	2:152:B:GLU:HA	8	0.36
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG13	3	0.36
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG11	4	0.36
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG12	6	0.36
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG11	9	0.36
(2,3205)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	2	0.36
(2,3120)	2:147:B:ASN:HB3	2:148:B:GLY:H	1	0.36
(2,3120)	2:147:B:ASN:HB2	2:148:B:GLY:H	7	0.36
(2,3099)	2:146:B:LEU:HD23	2:149:B:LYS:HE3	9	0.36
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB2	5	0.36
(2,2972)	2:134:B:ALA:HB2	2:139:B:LEU:HD22	6	0.36
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	5	0.36
(2,2703)	2:109:B:LEU:HD13	2:109:B:LEU:H	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2579)	1:61:A:CYS:HB3	1:62:A:ASN:HD21	3	0.36
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	6	0.36
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG21	4	0.36
(2,2260)	1:25:A:GLU:HG3	1:25:A:GLU:H	8	0.36
(2,2251)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	5	0.36
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	3	0.36
(2,2147)	1:15:A:ILE:HD11	2:103:B:TYR:HA	7	0.36
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	5	0.36
(2,2100)	1:10:A:ILE:HG23	1:47:A:PHE:HE2	8	0.36
(2,2004)	2:163:B:ALA:HB3	2:163:B:ALA:HA	6	0.36
(2,2004)	2:163:B:ALA:HB3	2:163:B:ALA:HA	10	0.36
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG3	9	0.36
(2,1881)	2:144:B:SER:HA	2:147:B:ASN:HB2	1	0.36
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	1	0.36
(2,1849)	2:139:B:LEU:HD22	2:124:B:LYS:HD2	8	0.36
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	5	0.36
(2,1712)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	2	0.36
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	2	0.36
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	7	0.36
(2,1708)	2:121:B:LYS:HA	2:121:B:LYS:HB3	8	0.36
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	4	0.36
(2,1614)	2:101:B:MET:HE2	1:14:A:LEU:HB2	4	0.36
(2,1399)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	2	0.36
(2,1391)	1:24:A:THR:HG23	1:27:A:LYS:HE3	4	0.36
(2,1384)	1:23:A:VAL:HG13	1:51:A:LEU:HD22	6	0.36
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	4	0.36
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	8	0.36
(2,1142)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	8	0.36
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	2	0.36
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	4	0.36
(2,736)	1:59:A:LEU:HD23	1:59:A:LEU:HG	2	0.36
(2,736)	1:59:A:LEU:HD23	1:59:A:LEU:HG	5	0.36
(2,736)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.36
(2,728)	1:54:A:VAL:HG22	1:58:A:SER:HB3	1	0.36
(2,682)	1:50:A:ALA:HB3	1:46:A:LEU:HB3	10	0.36
(2,637)	1:42:A:PHE:HB3	1:42:A:PHE:HD2	6	0.36
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	5	0.36
(2,493)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	4	0.36
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG22	3	0.36
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	6	0.36
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	7	0.36
(2,325)	2:161:B:LYS:H	2:161:B:LYS:HB2	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	9	0.36
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD11	1	0.36
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD2	3	0.36
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	1	0.36
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB3	8	0.36
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG12	6	0.36
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB2	5	0.36
(2,70)	1:26:A:ASP:H	1:25:A:GLU:HB2	10	0.36
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG22	3	0.36
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG22	10	0.36
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	6	0.36
(2,36)	1:13:A:ALA:H	1:59:A:LEU:HD11	6	0.36
(2,12)	1:3:A:SER:H	1:6:A:GLU:HG2	5	0.36
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	5	0.35
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD11	7	0.35
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	2	0.35
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	3	0.35
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD23	4	0.35
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD22	10	0.35
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD21	9	0.35
(2,3331)	1:14:A:LEU:HD23	2:159:B:ILE:HA	2	0.35
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	6	0.35
(2,3307)	1:4:A:VAL:HG22	2:112:B:LEU:HA	7	0.35
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG12	2	0.35
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG13	5	0.35
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG11	8	0.35
(2,3260)	2:163:B:ALA:HB2	2:163:B:ALA:HA	9	0.35
(2,3256)	2:162:B:LEU:HD11	2:159:B:ILE:HA	9	0.35
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	3	0.35
(2,3231)	2:159:B:ILE:HG22	2:159:B:ILE:H	4	0.35
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	3	0.35
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD11	7	0.35
(2,3062)	2:142:B:VAL:HG22	2:104:B:VAL:HA	10	0.35
(2,3054)	2:142:B:VAL:HG13	2:107:B:TYR:HD2	1	0.35
(2,2976)	2:134:B:ALA:HB3	2:135:B:ASP:HB2	4	0.35
(2,2849)	2:123:B:ILE:HG21	2:106:B:SER:HA	6	0.35
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB3	2	0.35
(2,2714)	2:110:B:ALA:HB1	2:123:B:ILE:H	7	0.35
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	5	0.35
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	8	0.35
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	2	0.35
(2,2456)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2456)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	10	0.35
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG22	5	0.35
(2,2346)	1:34:A:ALA:HB3	2:126:B:ILE:HG22	7	0.35
(2,2269)	1:26:A:ASP:HB3	1:27:A:LYS:H	1	0.35
(2,2267)	1:26:A:ASP:HB2	1:30:A:ALA:HB3	7	0.35
(2,2160)	1:16:A:LEU:HD12	1:21:A:VAL:H	3	0.35
(2,2160)	1:16:A:LEU:HD13	1:21:A:VAL:H	5	0.35
(2,2160)	1:16:A:LEU:HD11	1:21:A:VAL:H	7	0.35
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD12	5	0.35
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	2	0.35
(2,2147)	1:15:A:ILE:HD13	2:103:B:TYR:HA	1	0.35
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	8	0.35
(2,2004)	2:163:B:ALA:HB3	2:163:B:ALA:HA	2	0.35
(2,1992)	2:161:B:LYS:HE3	2:161:B:LYS:HD2	2	0.35
(2,1992)	2:161:B:LYS:HE3	2:161:B:LYS:HD2	8	0.35
(2,1885)	2:145:B:GLU:HA	2:145:B:GLU:HG2	4	0.35
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	6	0.35
(2,1856)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.35
(2,1856)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.35
(2,1856)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.35
(2,1809)	2:132:B:ILE:HG23	1:18:A:ASP:HB2	7	0.35
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	8	0.35
(2,1728)	2:123:B:ILE:HD12	2:139:B:LEU:HA	8	0.35
(2,1716)	2:121:B:LYS:HG2	2:121:B:LYS:HE2	9	0.35
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	1	0.35
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	3	0.35
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	7	0.35
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	8	0.35
(2,1613)	2:101:B:MET:HE2	2:101:B:MET:HG3	8	0.35
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	10	0.35
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG12	8	0.35
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	9	0.35
(2,1321)	1:7:A:LEU:HA	1:10:A:ILE:HG22	1	0.35
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	7	0.35
(2,1173)	2:154:B:VAL:HG11	2:146:B:LEU:HD11	4	0.35
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD11	7	0.35
(2,1090)	2:142:B:VAL:HG22	2:146:B:LEU:HD23	6	0.35
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD11	7	0.35
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	7	0.35
(2,1054)	2:139:B:LEU:HD22	2:124:B:LYS:HE2	3	0.35
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD13	2	0.35
(2,1051)	2:139:B:LEU:HA	2:141:B:LYS:HG2	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,937)	2:123:B:ILE:HG21	2:106:B:SER:HA	6	0.35
(2,866)	2:112:B:LEU:HD12	2:108:B:LEU:HB2	8	0.35
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	9	0.35
(2,736)	1:59:A:LEU:HD22	1:59:A:LEU:HG	3	0.35
(2,736)	1:59:A:LEU:HD13	1:59:A:LEU:HG	8	0.35
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG22	4	0.35
(2,707)	1:54:A:VAL:HG22	1:58:A:SER:HB3	1	0.35
(2,683)	1:50:A:ALA:HB1	1:54:A:VAL:HG12	4	0.35
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB2	6	0.35
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB2	7	0.35
(2,637)	1:42:A:PHE:HB3	1:42:A:PHE:HD2	4	0.35
(2,567)	1:34:A:ALA:HB3	2:126:B:ILE:HG22	7	0.35
(2,502)	1:26:A:ASP:HB2	1:30:A:ALA:HB3	7	0.35
(2,492)	1:25:A:GLU:HA	1:25:A:GLU:HG2	2	0.35
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG23	8	0.35
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG23	10	0.35
(2,474)	1:23:A:VAL:HA	1:51:A:LEU:HB2	6	0.35
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	3	0.35
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG11	9	0.35
(2,253)	2:128:B:ASP:H	2:125:B:LYS:HG2	10	0.35
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	3	0.35
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB3	10	0.35
(2,159)	1:63:A:VAL:H	1:62:A:ASN:HB2	2	0.35
(2,136)	1:51:A:LEU:H	1:50:A:ALA:HB2	7	0.35
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG23	2	0.35
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	4	0.35
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.34
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	10	0.34
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	7	0.34
(2,3507)	2:159:B:ILE:HG23	1:60:A:ILE:HG13	3	0.34
(2,3504)	1:59:A:LEU:HD11	2:159:B:ILE:HG22	2	0.34
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	7	0.34
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	5	0.34
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	5	0.34
(2,3393)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	9	0.34
(2,3261)	2:163:B:ALA:HB2	2:163:B:ALA:H	2	0.34
(2,3237)	2:161:B:LYS:HA	2:161:B:LYS:HG2	9	0.34
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	2	0.34
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	2	0.34
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	9	0.34
(2,3195)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	10	0.34
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD21	3	0.34
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD11	1	0.34
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD12	3	0.34
(2,3054)	2:142:B:VAL:HG13	2:107:B:TYR:HD2	7	0.34
(2,3050)	2:142:B:VAL:HA	2:142:B:VAL:HG21	8	0.34
(2,2982)	2:134:B:ALA:HB3	2:124:B:LYS:HA	7	0.34
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	5	0.34
(2,2945)	2:132:B:ILE:HD13	2:133:B:GLU:H	10	0.34
(2,2851)	2:123:B:ILE:HG22	2:126:B:ILE:H	8	0.34
(2,2842)	2:123:B:ILE:HG22	2:139:B:LEU:H	4	0.34
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB3	5	0.34
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB1	10	0.34
(2,2714)	2:110:B:ALA:HB1	2:123:B:ILE:H	1	0.34
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG11	1	0.34
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG12	4	0.34
(2,2456)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	3	0.34
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	5	0.34
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG22	1	0.34
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	1	0.34
(2,2328)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	9	0.34
(2,2324)	1:32:A:ILE:HD12	1:31:A:LEU:H	8	0.34
(2,2260)	1:25:A:GLU:HG3	1:25:A:GLU:H	6	0.34
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	5	0.34
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	8	0.34
(2,2160)	1:16:A:LEU:HD13	1:21:A:VAL:H	2	0.34
(2,2160)	1:16:A:LEU:HD11	1:21:A:VAL:H	8	0.34
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD12	2	0.34
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	7	0.34
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	3	0.34
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	6	0.34
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG11	1	0.34
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.34
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	3	0.34
(2,1898)	2:146:B:LEU:HD13	2:151:B:ILE:HG13	1	0.34
(2,1712)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	9	0.34
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	9	0.34
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	9	0.34
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG13	4	0.34
(2,1391)	1:24:A:THR:HG21	1:27:A:LYS:HE3	10	0.34
(2,1387)	1:23:A:VAL:HG13	1:48:A:ALA:HB2	10	0.34
(2,1244)	2:165:B:VAL:HB	2:165:B:VAL:HG13	7	0.34
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	2	0.34
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	1	0.34
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	3	0.34
(2,1028)	2:134:B:ALA:HB3	2:124:B:LYS:HA	7	0.34
(2,919)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	1	0.34
(2,827)	2:108:B:LEU:HD23	2:104:B:VAL:HB	10	0.34
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	2	0.34
(2,736)	1:59:A:LEU:HD13	1:59:A:LEU:HG	4	0.34
(2,736)	1:59:A:LEU:HD12	1:59:A:LEU:HG	6	0.34
(2,736)	1:59:A:LEU:HD13	1:59:A:LEU:HG	9	0.34
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG21	9	0.34
(2,695)	1:51:A:LEU:HD12	1:48:A:ALA:HA	10	0.34
(2,692)	1:51:A:LEU:HD13	1:13:A:ALA:HB1	6	0.34
(2,587)	1:37:A:VAL:HG23	2:112:B:LEU:HD21	8	0.34
(2,492)	1:25:A:GLU:HA	1:25:A:GLU:HG2	9	0.34
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG21	1	0.34
(2,434)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	9	0.34
(2,422)	1:15:A:ILE:HD11	2:106:B:SER:HB2	6	0.34
(2,422)	1:15:A:ILE:HD11	2:106:B:SER:HB2	10	0.34
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	3	0.34
(2,332)	2:165:B:VAL:H	2:164:B:SER:HB2	8	0.34
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	1	0.34
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD13	9	0.34
(2,253)	2:128:B:ASP:H	2:124:B:LYS:HD2	2	0.34
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE2	5	0.34
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG12	9	0.34
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG13	8	0.34
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD11	6	0.34
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	6	0.34
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	7	0.34
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG22	9	0.34
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	2	0.33
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	4	0.33
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	2	0.33
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	4	0.33
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	7	0.33
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	8	0.33
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	10	0.33
(2,3858)	2:125:B:LYS:H	2:125:B:LYS:HB2	10	0.33
(2,3507)	2:159:B:ILE:HG23	1:60:A:ILE:HG13	5	0.33
(2,3507)	2:159:B:ILE:HG21	1:60:A:ILE:HG13	10	0.33
(2,3497)	1:59:A:LEU:HD11	2:159:B:ILE:HB	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	6	0.33
(2,3493)	2:152:B:GLU:HG2	1:4:A:VAL:HB	7	0.33
(2,3405)	1:59:A:LEU:HD11	2:159:B:ILE:HB	2	0.33
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	6	0.33
(2,3403)	1:59:A:LEU:HD11	2:159:B:ILE:HB	2	0.33
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	6	0.33
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	3	0.33
(2,3402)	1:59:A:LEU:HD12	2:159:B:ILE:HA	8	0.33
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	3	0.33
(2,3399)	1:59:A:LEU:HD12	2:159:B:ILE:HA	8	0.33
(2,3364)	1:31:A:LEU:HD13	2:130:B:VAL:HA	8	0.33
(2,3331)	1:14:A:LEU:HD23	2:159:B:ILE:HA	1	0.33
(2,3331)	1:14:A:LEU:HD22	2:159:B:ILE:HA	4	0.33
(2,3298)	1:1:A:MET:HG3	2:153:B:ASP:HB2	10	0.33
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	9	0.33
(2,3260)	2:163:B:ALA:HB1	2:163:B:ALA:HA	8	0.33
(2,3231)	2:159:B:ILE:HG23	2:159:B:ILE:H	2	0.33
(2,3231)	2:159:B:ILE:HG21	2:159:B:ILE:H	8	0.33
(2,3231)	2:159:B:ILE:HG23	2:159:B:ILE:H	9	0.33
(2,3205)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	9	0.33
(2,3178)	2:154:B:VAL:H	2:154:B:VAL:HG23	10	0.33
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.33
(2,3131)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	6	0.33
(2,3120)	2:147:B:ASN:HB3	2:148:B:GLY:H	5	0.33
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	9	0.33
(2,3055)	2:142:B:VAL:HA	2:142:B:VAL:HG21	9	0.33
(2,3029)	2:139:B:LEU:HD21	2:124:B:LYS:HA	6	0.33
(2,2982)	2:134:B:ALA:HB1	2:124:B:LYS:HA	2	0.33
(2,2982)	2:134:B:ALA:HB1	2:124:B:LYS:HA	5	0.33
(2,2851)	2:123:B:ILE:HG22	2:126:B:ILE:H	1	0.33
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB3	7	0.33
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB3	8	0.33
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB3	9	0.33
(2,2717)	2:110:B:ALA:HB2	2:115:B:ASN:HD21	1	0.33
(2,2714)	2:110:B:ALA:HB1	2:123:B:ILE:H	10	0.33
(2,2703)	2:109:B:LEU:HD13	2:109:B:LEU:H	7	0.33
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG12	3	0.33
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG11	6	0.33
(2,2498)	1:51:A:LEU:HD13	1:13:A:ALA:HB1	6	0.33
(2,2372)	1:37:A:VAL:HG21	2:112:B:LEU:HG	5	0.33
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG23	2	0.33
(2,2328)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2269)	1:26:A:ASP:HB3	1:27:A:LYS:H	4	0.33
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	1	0.33
(2,2204)	1:20:A:GLU:HG3	1:19:A:ASP:H	2	0.33
(2,2160)	1:16:A:LEU:HD13	1:21:A:VAL:H	6	0.33
(2,2094)	1:10:A:ILE:HD13	1:7:A:LEU:H	8	0.33
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	5	0.33
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	8	0.33
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	9	0.33
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG13	3	0.33
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG11	4	0.33
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG12	6	0.33
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG11	9	0.33
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	3	0.33
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	7	0.33
(2,1864)	2:142:B:VAL:HA	2:142:B:VAL:HG21	8	0.33
(2,1851)	2:139:B:LEU:HD12	2:120:B:ALA:HA	2	0.33
(2,1659)	2:111:B:ALA:HB1	2:151:B:ILE:HD12	1	0.33
(2,1659)	2:111:B:ALA:HB3	2:151:B:ILE:HD12	6	0.33
(2,1641)	2:108:B:LEU:HD21	2:155:B:ILE:HG21	1	0.33
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	7	0.33
(2,1629)	2:105:B:ALA:HB2	2:101:B:MET:HG2	6	0.33
(2,1625)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	5	0.33
(2,1613)	2:101:B:MET:HE2	2:101:B:MET:HG2	5	0.33
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	1	0.33
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	4	0.33
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG11	7	0.33
(2,1384)	1:23:A:VAL:HG12	1:51:A:LEU:HD13	8	0.33
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	1	0.33
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	2	0.33
(2,1307)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	2	0.33
(2,1186)	2:156:B:ALA:HB1	2:157:B:GLN:HG2	10	0.33
(2,1082)	2:142:B:VAL:HG12	2:103:B:TYR:HD2	9	0.33
(2,1056)	2:139:B:LEU:HD12	2:120:B:ALA:HA	4	0.33
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD11	6	0.33
(2,1033)	2:134:B:ALA:HB2	2:139:B:LEU:HD22	6	0.33
(2,1028)	2:134:B:ALA:HB1	2:124:B:LYS:HA	2	0.33
(2,1028)	2:134:B:ALA:HB1	2:124:B:LYS:HA	5	0.33
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG23	3	0.33
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	2	0.33
(2,498)	1:25:A:GLU:HG3	1:48:A:ALA:HB3	3	0.33
(2,497)	1:25:A:GLU:HA	1:25:A:GLU:HG2	5	0.33
(2,493)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG21	7	0.33
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG22	9	0.33
(2,414)	1:14:A:LEU:HD12	2:101:B:MET:HG3	3	0.33
(2,357)	1:4:A:VAL:HG23	2:112:B:LEU:HA	8	0.33
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	1	0.33
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	9	0.33
(2,317)	2:154:B:VAL:H	2:154:B:VAL:HG23	3	0.33
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	6	0.33
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	3	0.33
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG12	5	0.33
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG13	8	0.33
(2,279)	2:139:B:LEU:H	2:139:B:LEU:HD13	3	0.33
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD13	7	0.33
(2,188)	2:112:B:LEU:H	1:37:A:VAL:HG11	10	0.33
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB3	1	0.33
(2,139)	1:53:A:ASN:H	1:54:A:VAL:HG22	7	0.33
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD13	6	0.33
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG21	1	0.33
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG22	8	0.33
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD11	1	0.33
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	7	0.32
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	8	0.32
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	10	0.32
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	1	0.32
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	3	0.32
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	6	0.32
(2,4159)	1:56:A:ILE:HG12	1:56:A:ILE:HA	7	0.32
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	9	0.32
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	1	0.32
(2,3507)	2:159:B:ILE:HG23	1:60:A:ILE:HG13	1	0.32
(2,3507)	2:159:B:ILE:HG21	1:60:A:ILE:HG13	7	0.32
(2,3396)	1:39:A:VAL:HG21	2:109:B:LEU:HD13	3	0.32
(2,3388)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	9	0.32
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	5	0.32
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	9	0.32
(2,3305)	1:4:A:VAL:HG11	2:112:B:LEU:HA	5	0.32
(2,3296)	1:1:A:MET:HE3	2:156:B:ALA:HA	10	0.32
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	5	0.32
(2,3271)	2:165:B:VAL:HB	2:165:B:VAL:HG13	7	0.32
(2,3260)	2:163:B:ALA:HB1	2:163:B:ALA:HA	3	0.32
(2,3260)	2:163:B:ALA:HB1	2:163:B:ALA:HA	7	0.32
(2,3178)	2:154:B:VAL:H	2:154:B:VAL:HG23	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3123)	2:147:B:ASN:HB3	2:148:B:GLY:H	4	0.32
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG21	3	0.32
(2,3049)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	1	0.32
(2,3049)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	3	0.32
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB3	3	0.32
(2,2945)	2:132:B:ILE:HD13	2:133:B:GLU:H	6	0.32
(2,2851)	2:123:B:ILE:HG22	2:126:B:ILE:H	10	0.32
(2,2850)	2:123:B:ILE:HG23	2:139:B:LEU:HA	3	0.32
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB3	4	0.32
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB3	9	0.32
(2,2742)	1:37:A:VAL:HG22	2:112:B:LEU:HD23	2	0.32
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB2	7	0.32
(2,2713)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	6	0.32
(2,2558)	1:59:A:LEU:HD22	1:59:A:LEU:HG	7	0.32
(2,2558)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.32
(2,2388)	1:37:A:VAL:HG22	1:38:A:ASN:HB3	4	0.32
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	10	0.32
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	2	0.32
(2,2286)	1:28:A:ILE:HD12	1:44:A:PRO:HA	9	0.32
(2,2251)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	9	0.32
(2,2251)	1:25:A:GLU:HB3	1:48:A:ALA:HB1	10	0.32
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	1	0.32
(2,2160)	1:16:A:LEU:HD13	1:21:A:VAL:H	9	0.32
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	9	0.32
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG12	2	0.32
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG13	5	0.32
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG11	8	0.32
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	5	0.32
(2,1992)	2:161:B:LYS:HE3	2:161:B:LYS:HD2	3	0.32
(2,1989)	2:161:B:LYS:HA	2:161:B:LYS:HG2	6	0.32
(2,1962)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	9	0.32
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	6	0.32
(2,1721)	2:122:B:ASP:HA	2:125:B:LYS:HG3	10	0.32
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	6	0.32
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	10	0.32
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	4	0.32
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	6	0.32
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG2	4	0.32
(2,1532)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	9	0.32
(2,1510)	1:28:A:ILE:HD12	1:44:A:PRO:HA	9	0.32
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	1	0.32
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	8	0.32
(2,1269)	1:2:A:ALA:HA	1:2:A:ALA:HB2	10	0.32
(2,1219)	2:161:B:LYS:HA	2:161:B:LYS:HG2	6	0.32
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	8	0.32
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	10	0.32
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD22	4	0.32
(2,1081)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	1	0.32
(2,1081)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	3	0.32
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	5	0.32
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	8	0.32
(2,1042)	2:137:B:ASP:HA	2:139:B:LEU:HD13	10	0.32
(2,683)	1:50:A:ALA:HB3	1:54:A:VAL:HG11	8	0.32
(2,657)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	2	0.32
(2,657)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	8	0.32
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD2	4	0.32
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD2	6	0.32
(2,522)	1:28:A:ILE:HD12	1:44:A:PRO:HA	9	0.32
(2,498)	1:25:A:GLU:HG2	1:48:A:ALA:HB3	9	0.32
(2,422)	1:15:A:ILE:HD11	2:106:B:SER:HB2	3	0.32
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	10	0.32
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	2	0.32
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	7	0.32
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	2	0.32
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB2	5	0.32
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD22	6	0.32
(2,159)	1:63:A:VAL:H	1:62:A:ASN:HB3	8	0.32
(2,70)	1:26:A:ASP:H	1:25:A:GLU:HB2	5	0.32
(2,69)	1:26:A:ASP:H	1:24:A:THR:HG22	4	0.32
(2,61)	1:24:A:THR:H	1:23:A:VAL:HG12	2	0.32
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	2	0.31
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	4	0.31
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	9	0.31
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	1	0.31
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	2	0.31
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	5	0.31
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	8	0.31
(2,4203)	2:155:B:ILE:HD12	2:155:B:ILE:HB	8	0.31
(2,4181)	2:124:B:LYS:HA	2:124:B:LYS:HD2	5	0.31
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	6	0.31
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	5	0.31
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	8	0.31
(2,3507)	2:159:B:ILE:HG21	1:60:A:ILE:HG13	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3507)	2:159:B:ILE:HG21	1:60:A:ILE:HG13	8	0.31
(2,3497)	1:59:A:LEU:HD11	2:159:B:ILE:HB	1	0.31
(2,3492)	2:152:B:GLU:HG2	1:7:A:LEU:HB3	7	0.31
(2,3469)	2:130:B:VAL:HG21	1:16:A:LEU:HB2	6	0.31
(2,3416)	2:101:B:MET:HE1	1:17:A:HIS:HD2	5	0.31
(2,3405)	1:59:A:LEU:HD11	2:159:B:ILE:HB	1	0.31
(2,3403)	1:59:A:LEU:HD11	2:159:B:ILE:HB	1	0.31
(2,3396)	1:39:A:VAL:HG21	2:109:B:LEU:HD12	6	0.31
(2,3336)	1:15:A:ILE:HD11	2:109:B:LEU:HD23	5	0.31
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	9	0.31
(2,3261)	2:163:B:ALA:HB2	2:163:B:ALA:H	5	0.31
(2,3261)	2:163:B:ALA:HB2	2:163:B:ALA:H	6	0.31
(2,3247)	2:162:B:LEU:H	2:162:B:LEU:HB2	5	0.31
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	1	0.31
(2,3234)	2:159:B:ILE:HG21	1:61:A:CYS:H	7	0.31
(2,3234)	2:159:B:ILE:HG21	1:61:A:CYS:H	8	0.31
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	2	0.31
(2,3231)	2:159:B:ILE:HG23	2:159:B:ILE:H	1	0.31
(2,3231)	2:159:B:ILE:HG21	2:159:B:ILE:H	10	0.31
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	6	0.31
(2,3054)	2:142:B:VAL:HG12	2:107:B:TYR:HD2	8	0.31
(2,3049)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	5	0.31
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	5	0.31
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	5	0.31
(2,2969)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.31
(2,2916)	2:128:B:ASP:HB2	2:124:B:LYS:HB3	8	0.31
(2,2822)	2:120:B:ALA:HB3	2:140:B:ASN:H	7	0.31
(2,2822)	2:120:B:ALA:HB3	2:140:B:ASN:H	8	0.31
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB3	5	0.31
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB3	4	0.31
(2,2713)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	5	0.31
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	3	0.31
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	10	0.31
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG12	8	0.31
(2,2645)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	5	0.31
(2,2558)	1:59:A:LEU:HD23	1:59:A:LEU:HG	2	0.31
(2,2558)	1:59:A:LEU:HD22	1:59:A:LEU:HG	3	0.31
(2,2558)	1:59:A:LEU:HD23	1:59:A:LEU:HG	5	0.31
(2,2558)	1:59:A:LEU:HD13	1:59:A:LEU:HG	8	0.31
(2,2384)	1:37:A:VAL:HA	1:38:A:ASN:HB2	8	0.31
(2,2372)	1:37:A:VAL:HG22	2:112:B:LEU:HG	2	0.31
(2,2368)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	2	0.31
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	8	0.31
(2,2304)	1:30:A:ALA:HA	1:33:A:LYS:HD3	9	0.31
(2,2261)	1:25:A:GLU:HG2	1:26:A:ASP:H	4	0.31
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG11	7	0.31
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG11	8	0.31
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG13	10	0.31
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	5	0.31
(2,2209)	1:21:A:VAL:HG12	1:19:A:ASP:H	7	0.31
(2,2166)	1:16:A:LEU:HD12	1:27:A:LYS:HE3	7	0.31
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD11	3	0.31
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG13	4	0.31
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB3	1	0.31
(2,1946)	2:154:B:VAL:HG23	2:149:B:LYS:HG2	10	0.31
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	3	0.31
(2,1885)	2:145:B:GLU:HA	2:145:B:GLU:HG2	9	0.31
(2,1881)	2:144:B:SER:HA	2:147:B:ASN:HB2	4	0.31
(2,1857)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.31
(2,1857)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.31
(2,1857)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.31
(2,1765)	2:126:B:ILE:HD12	2:125:B:LYS:HD3	2	0.31
(2,1712)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	1	0.31
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD2	10	0.31
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	1	0.31
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	3	0.31
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	8	0.31
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD11	1	0.31
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	7	0.31
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	10	0.31
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG11	1	0.31
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG13	3	0.31
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB1	9	0.31
(2,1351)	1:16:A:LEU:HD21	1:23:A:VAL:HG23	7	0.31
(2,1314)	1:10:A:ILE:HB	1:10:A:ILE:HD11	3	0.31
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	3	0.31
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	1	0.31
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	3	0.31
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	4	0.31
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	5	0.31
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	6	0.31
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	9	0.31
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB1	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	9	0.31
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	4	0.31
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	4	0.31
(2,1082)	2:142:B:VAL:HG12	2:103:B:TYR:HD2	4	0.31
(2,1082)	2:142:B:VAL:HG13	2:103:B:TYR:HD2	5	0.31
(2,1081)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	5	0.31
(2,919)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	7	0.31
(2,795)	2:104:B:VAL:HG22	2:103:B:TYR:HA	2	0.31
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	1	0.31
(2,736)	1:59:A:LEU:HD12	1:59:A:LEU:HG	1	0.31
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG22	8	0.31
(2,682)	1:50:A:ALA:HB2	1:46:A:LEU:HB2	6	0.31
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	7	0.31
(2,657)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	1	0.31
(2,657)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	5	0.31
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	8	0.31
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	10	0.31
(2,530)	1:30:A:ALA:HA	1:33:A:LYS:HD3	9	0.31
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG22	4	0.31
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	6	0.31
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	10	0.31
(2,327)	2:162:B:LEU:H	2:162:B:LEU:HB2	5	0.31
(2,314)	2:153:B:ASP:H	2:154:B:VAL:HG21	1	0.31
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG11	4	0.31
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG12	10	0.31
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB3	5	0.31
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	6	0.31
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG13	2	0.31
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG13	10	0.31
(2,70)	1:26:A:ASP:H	1:25:A:GLU:HB2	2	0.31
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD13	1	0.31
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD13	5	0.31
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	6	0.31
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	6	0.3
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	3	0.3
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	4	0.3
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	7	0.3
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	10	0.3
(2,4193)	2:140:B:ASN:HA	2:143:B:ILE:HD13	5	0.3
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	1	0.3
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	3	0.3
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	6	0.3
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	6	0.3
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	9	0.3
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	3	0.3
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD21	1	0.3
(2,3413)	2:101:B:MET:HE2	1:14:A:LEU:HB2	8	0.3
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	3	0.3
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	3	0.3
(2,3331)	1:14:A:LEU:HD21	2:159:B:ILE:HA	9	0.3
(2,3331)	1:14:A:LEU:HD21	2:159:B:ILE:HA	10	0.3
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	1	0.3
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	8	0.3
(2,3261)	2:163:B:ALA:HB3	2:163:B:ALA:H	3	0.3
(2,3260)	2:163:B:ALA:HB3	2:163:B:ALA:HA	1	0.3
(2,3253)	2:162:B:LEU:HD23	2:162:B:LEU:HG	8	0.3
(2,3247)	2:162:B:LEU:H	2:162:B:LEU:HB2	9	0.3
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG22	5	0.3
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG23	6	0.3
(2,3231)	2:159:B:ILE:HG21	2:159:B:ILE:H	6	0.3
(2,3172)	2:154:B:VAL:HG13	2:155:B:ILE:H	1	0.3
(2,3068)	2:140:B:ASN:HA	2:143:B:ILE:HD13	5	0.3
(2,3013)	2:139:B:LEU:H	2:139:B:LEU:HD13	3	0.3
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	6	0.3
(2,2970)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.3
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	6	0.3
(2,2945)	2:132:B:ILE:HD12	2:133:B:GLU:H	1	0.3
(2,2860)	2:124:B:LYS:HG2	2:124:B:LYS:HE3	5	0.3
(2,2808)	2:119:B:SER:HB2	2:121:B:LYS:HD3	5	0.3
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB2	6	0.3
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB3	6	0.3
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	1	0.3
(2,2558)	1:59:A:LEU:HD12	1:59:A:LEU:HG	6	0.3
(2,2558)	1:59:A:LEU:HD13	1:59:A:LEU:HG	9	0.3
(2,2540)	1:54:A:VAL:HG22	1:58:A:SER:HB3	1	0.3
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	3	0.3
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	1	0.3
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	7	0.3
(2,2372)	1:37:A:VAL:HG23	2:112:B:LEU:HG	8	0.3
(2,2372)	1:37:A:VAL:HG21	2:112:B:LEU:HG	9	0.3
(2,2372)	1:37:A:VAL:HG22	2:112:B:LEU:HG	10	0.3
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG23	10	0.3
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2261)	1:25:A:GLU:HG2	1:26:A:ASP:H	1	0.3
(2,2260)	1:25:A:GLU:HG3	1:25:A:GLU:H	3	0.3
(2,2258)	1:25:A:GLU:HG3	1:48:A:ALA:HB1	8	0.3
(2,2250)	1:25:A:GLU:HB3	1:28:A:ILE:H	1	0.3
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	5	0.3
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	9	0.3
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	3	0.3
(2,2165)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	9	0.3
(2,2160)	1:16:A:LEU:HD13	1:21:A:VAL:H	4	0.3
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG22	5	0.3
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	1	0.3
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	4	0.3
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG22	9	0.3
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	1	0.3
(2,1842)	2:139:B:LEU:HD12	2:120:B:ALA:HA	2	0.3
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB2	5	0.3
(2,1716)	2:121:B:LYS:HG2	2:121:B:LYS:HE2	2	0.3
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	2	0.3
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	5	0.3
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	10	0.3
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	10	0.3
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	5	0.3
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	9	0.3
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG12	2	0.3
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG11	6	0.3
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG13	9	0.3
(2,1381)	1:23:A:VAL:HG13	1:48:A:ALA:HB2	10	0.3
(2,1314)	1:10:A:ILE:HB	1:10:A:ILE:HD11	1	0.3
(2,1314)	1:10:A:ILE:HB	1:10:A:ILE:HD11	8	0.3
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	1	0.3
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB2	4	0.3
(2,1234)	2:163:B:ALA:HB2	2:163:B:ALA:HA	9	0.3
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	9	0.3
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	1	0.3
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	2	0.3
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	7	0.3
(2,1207)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.3
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	2	0.3
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	7	0.3
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	3	0.3
(2,1162)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	7	0.3
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	7	0.3
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	1	0.3
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	10	0.3
(2,1103)	2:140:B:ASN:HA	2:143:B:ILE:HD13	5	0.3
(2,1082)	2:142:B:VAL:HG12	2:103:B:TYR:HD2	7	0.3
(2,1082)	2:142:B:VAL:HG11	2:103:B:TYR:HD2	8	0.3
(2,1071)	2:140:B:ASN:HA	2:143:B:ILE:HD13	5	0.3
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	9	0.3
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	10	0.3
(2,919)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	10	0.3
(2,728)	1:54:A:VAL:HG21	1:58:A:SER:HB3	4	0.3
(2,695)	1:51:A:LEU:HD12	1:48:A:ALA:HA	9	0.3
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	8	0.3
(2,657)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	7	0.3
(2,587)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	4	0.3
(2,497)	1:25:A:GLU:HA	1:25:A:GLU:HG2	10	0.3
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG22	5	0.3
(2,439)	1:16:A:LEU:HD23	1:13:A:ALA:HA	4	0.3
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	7	0.3
(2,422)	1:15:A:ILE:HD11	2:106:B:SER:HB2	7	0.3
(2,389)	1:10:A:ILE:HD11	1:7:A:LEU:HG	9	0.3
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	6	0.3
(2,357)	1:4:A:VAL:HG11	2:112:B:LEU:HA	6	0.3
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	5	0.3
(2,329)	2:164:B:SER:H	2:162:B:LEU:HB3	4	0.3
(2,328)	2:163:B:ALA:H	2:162:B:LEU:HB3	1	0.3
(2,327)	2:162:B:LEU:H	2:162:B:LEU:HB2	9	0.3
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	8	0.3
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	4	0.3
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG11	1	0.3
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD12	3	0.3
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	6	0.3
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE2	8	0.3
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	3	0.3
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB1	4	0.3
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	3	0.3
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	4	0.3
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG12	5	0.3
(2,169)	1:43:A:TRP:HE1	1:5:A:SER:HB2	1	0.3
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD13	1	0.3
(2,126)	1:47:A:PHE:H	1:46:A:LEU:HD13	8	0.3
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD12	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD13	7	0.3
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD13	8	0.3
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD22	10	0.3
(2,12)	1:3:A:SER:H	1:6:A:GLU:HG2	9	0.3
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	9	0.3
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	1	0.29
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	6	0.29
(2,4528)	2:151:B:ILE:HA	2:151:B:ILE:HG12	9	0.29
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	4	0.29
(2,4181)	2:124:B:LYS:HA	2:124:B:LYS:HD2	6	0.29
(2,4122)	2:159:B:ILE:HA	2:159:B:ILE:HG12	5	0.29
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	8	0.29
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	4	0.29
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	3	0.29
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	5	0.29
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	7	0.29
(2,3494)	1:7:A:LEU:HD13	2:155:B:ILE:HG22	3	0.29
(2,3445)	2:112:B:LEU:HA	1:37:A:VAL:HG21	1	0.29
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	7	0.29
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	7	0.29
(2,3393)	1:37:A:VAL:HG11	2:109:B:LEU:HD11	2	0.29
(2,3332)	1:14:A:LEU:HD12	2:101:B:MET:HG3	8	0.29
(2,3331)	1:14:A:LEU:HD23	2:159:B:ILE:HA	3	0.29
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	2	0.29
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	7	0.29
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG22	10	0.29
(2,3305)	1:4:A:VAL:HG11	2:112:B:LEU:HA	10	0.29
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	5	0.29
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	3	0.29
(2,3260)	2:163:B:ALA:HB3	2:163:B:ALA:HA	4	0.29
(2,3260)	2:163:B:ALA:HB3	2:163:B:ALA:HA	5	0.29
(2,3253)	2:162:B:LEU:HD12	2:162:B:LEU:HG	6	0.29
(2,3237)	2:161:B:LYS:HA	2:161:B:LYS:HG2	6	0.29
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	9	0.29
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	1	0.29
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG22	1	0.29
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG22	3	0.29
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	4	0.29
(2,3178)	2:154:B:VAL:H	2:154:B:VAL:HG23	2	0.29
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	3	0.29
(2,3109)	2:104:B:VAL:HG21	2:146:B:LEU:HD22	10	0.29
(2,3054)	2:142:B:VAL:HG13	2:107:B:TYR:HD2	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	10	0.29
(2,3004)	2:138:B:ARG:HB3	2:138:B:ARG:HD2	6	0.29
(2,2970)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	7	0.29
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	8	0.29
(2,2969)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	7	0.29
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	8	0.29
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	2	0.29
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	3	0.29
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	5	0.29
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	6	0.29
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	7	0.29
(2,2768)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	6	0.29
(2,2688)	2:108:B:LEU:HD13	2:155:B:ILE:H	4	0.29
(2,2628)	2:101:B:MET:HE3	2:103:B:TYR:HA	3	0.29
(2,2601)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	3	0.29
(2,2589)	1:62:A:ASN:HB2	1:43:A:TRP:HZ2	1	0.29
(2,2558)	1:59:A:LEU:HD13	1:59:A:LEU:HG	4	0.29
(2,2431)	1:42:A:PHE:HB3	1:42:A:PHE:HD2	6	0.29
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	2	0.29
(2,2405)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	2	0.29
(2,2372)	1:37:A:VAL:HG21	2:112:B:LEU:HG	3	0.29
(2,2372)	1:37:A:VAL:HG23	2:112:B:LEU:HG	4	0.29
(2,2372)	1:37:A:VAL:HG22	2:112:B:LEU:HG	6	0.29
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG21	8	0.29
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG22	9	0.29
(2,2285)	1:28:A:ILE:HA	1:31:A:LEU:HD22	10	0.29
(2,2269)	1:26:A:ASP:HB3	1:27:A:LYS:H	2	0.29
(2,2256)	1:25:A:GLU:HG2	1:29:A:ASN:HD21	1	0.29
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	3	0.29
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	2	0.29
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	8	0.29
(2,2209)	1:21:A:VAL:HG12	1:19:A:ASP:H	1	0.29
(2,2209)	1:21:A:VAL:HG12	1:19:A:ASP:H	2	0.29
(2,2166)	1:16:A:LEU:HD12	1:27:A:LYS:HE3	10	0.29
(2,2152)	1:15:A:ILE:HG23	2:103:B:TYR:HA	4	0.29
(2,2057)	1:4:A:VAL:HG11	2:112:B:LEU:HB3	1	0.29
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG21	4	0.29
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG23	7	0.29
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG21	9	0.29
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	10	0.29
(2,2012)	2:165:B:VAL:HB	2:165:B:VAL:HG13	7	0.29
(2,1989)	2:161:B:LYS:HA	2:161:B:LYS:HG2	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1934)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	7	0.29
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	2	0.29
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	3	0.29
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	5	0.29
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	8	0.29
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	9	0.29
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB3	10	0.29
(2,1742)	2:134:B:ALA:HB3	2:124:B:LYS:HA	3	0.29
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB2	7	0.29
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB3	4	0.29
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	2	0.29
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	4	0.29
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	6	0.29
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	9	0.29
(2,1614)	2:101:B:MET:HE1	1:14:A:LEU:HB2	5	0.29
(2,1613)	2:101:B:MET:HE3	2:101:B:MET:HG2	3	0.29
(2,1561)	1:56:A:ILE:HD11	1:10:A:ILE:HG21	2	0.29
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	5	0.29
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	6	0.29
(2,1532)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	7	0.29
(2,1497)	1:41:A:PRO:HA	1:41:A:PRO:HD3	3	0.29
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG11	10	0.29
(2,1399)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	5	0.29
(2,1391)	1:24:A:THR:HG21	1:27:A:LYS:HE3	6	0.29
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	5	0.29
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	7	0.29
(2,1314)	1:10:A:ILE:HB	1:10:A:ILE:HD11	6	0.29
(2,1219)	2:161:B:LYS:HA	2:161:B:LYS:HG2	5	0.29
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	8	0.29
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	1	0.29
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	3	0.29
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	6	0.29
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	9	0.29
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	3	0.29
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	4	0.29
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD12	8	0.29
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	5	0.29
(2,920)	2:122:B:ASP:HA	2:125:B:LYS:HG3	10	0.29
(2,919)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	8	0.29
(2,866)	2:112:B:LEU:HD21	2:108:B:LEU:HB2	1	0.29
(2,842)	2:109:B:LEU:HD22	1:12:A:SER:HA	9	0.29
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	7	0.29
(2,774)	2:101:B:MET:HE3	2:103:B:TYR:HA	3	0.29
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG21	5	0.29
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG22	7	0.29
(2,707)	1:54:A:VAL:HG21	1:58:A:SER:HB3	4	0.29
(2,683)	1:50:A:ALA:HB2	1:54:A:VAL:HG22	1	0.29
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	1	0.29
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	4	0.29
(2,680)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	9	0.29
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	6	0.29
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	1	0.29
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	4	0.29
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	10	0.29
(2,660)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	1	0.29
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG12	8	0.29
(2,596)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	7	0.29
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	2	0.29
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	7	0.29
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	8	0.29
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	8	0.29
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	6	0.29
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	7	0.29
(2,329)	2:164:B:SER:H	2:162:B:LEU:HB3	6	0.29
(2,328)	2:163:B:ALA:H	2:162:B:LEU:HB3	8	0.29
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	6	0.29
(2,275)	2:136:B:ASP:H	2:135:B:ASP:HB2	6	0.29
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	5	0.29
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	9	0.29
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG23	1	0.29
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	10	0.29
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	3	0.28
(2,4555)	2:159:B:ILE:HA	2:159:B:ILE:HG12	5	0.28
(2,4186)	2:127:B:LEU:HG	2:124:B:LYS:HD2	5	0.28
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG13	9	0.28
(2,3507)	2:159:B:ILE:HG22	1:60:A:ILE:HG13	4	0.28
(2,3507)	2:159:B:ILE:HG23	1:60:A:ILE:HG13	9	0.28
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	7	0.28
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	9	0.28
(2,3493)	2:152:B:GLU:HG3	1:4:A:VAL:HB	1	0.28
(2,3493)	2:152:B:GLU:HG2	1:4:A:VAL:HB	3	0.28
(2,3435)	1:15:A:ILE:HD11	2:109:B:LEU:HD23	8	0.28
(2,3408)	1:60:A:ILE:HD13	2:157:B:GLN:HB3	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	9	0.28
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	9	0.28
(2,3364)	1:31:A:LEU:HD11	2:130:B:VAL:HA	1	0.28
(2,3331)	1:14:A:LEU:HD23	2:159:B:ILE:HA	8	0.28
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	3	0.28
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	8	0.28
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	10	0.28
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG21	2	0.28
(2,3301)	1:2:A:ALA:HB1	2:152:B:GLU:HA	2	0.28
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	1	0.28
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	8	0.28
(2,3261)	2:163:B:ALA:HB2	2:163:B:ALA:H	10	0.28
(2,3260)	2:163:B:ALA:HB3	2:163:B:ALA:HA	6	0.28
(2,3260)	2:163:B:ALA:HB3	2:163:B:ALA:HA	10	0.28
(2,3253)	2:162:B:LEU:HD11	2:162:B:LEU:HG	2	0.28
(2,3253)	2:162:B:LEU:HD22	2:162:B:LEU:HG	3	0.28
(2,3253)	2:162:B:LEU:HD12	2:162:B:LEU:HG	4	0.28
(2,3235)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	4	0.28
(2,3120)	2:147:B:ASN:HB2	2:148:B:GLY:H	6	0.28
(2,3054)	2:142:B:VAL:HG11	2:107:B:TYR:HD2	5	0.28
(2,3049)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	4	0.28
(2,3043)	2:141:B:LYS:HA	2:144:B:SER:H	2	0.28
(2,3043)	2:141:B:LYS:HA	2:144:B:SER:H	5	0.28
(2,3018)	2:139:B:LEU:HD12	2:138:B:ARG:H	8	0.28
(2,2982)	2:134:B:ALA:HB3	2:124:B:LYS:HA	9	0.28
(2,2982)	2:134:B:ALA:HB1	2:124:B:LYS:HA	10	0.28
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	3	0.28
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	9	0.28
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	9	0.28
(2,2946)	2:132:B:ILE:HD12	1:20:A:GLU:H	9	0.28
(2,2855)	2:124:B:LYS:HA	2:124:B:LYS:HE3	1	0.28
(2,2851)	2:123:B:ILE:HG22	2:126:B:ILE:H	2	0.28
(2,2842)	2:123:B:ILE:HG23	2:139:B:LEU:H	1	0.28
(2,2808)	2:119:B:SER:HB2	2:121:B:LYS:HD3	1	0.28
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB1	1	0.28
(2,2732)	2:117:B:SER:H	2:111:B:ALA:HB1	3	0.28
(2,2717)	2:110:B:ALA:HB2	2:115:B:ASN:HD21	3	0.28
(2,2717)	2:110:B:ALA:HB1	2:115:B:ASN:HD21	8	0.28
(2,2709)	2:109:B:LEU:HD22	1:12:A:SER:HA	9	0.28
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG11	7	0.28
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	5	0.28
(2,2527)	1:56:A:ILE:HD12	1:17:A:HIS:HD2	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2431)	1:42:A:PHE:HB3	1:42:A:PHE:HD2	4	0.28
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	5	0.28
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	3	0.28
(2,2372)	1:37:A:VAL:HG21	2:112:B:LEU:HG	1	0.28
(2,2372)	1:37:A:VAL:HG23	2:112:B:LEU:HG	7	0.28
(2,2267)	1:26:A:ASP:HB2	1:30:A:ALA:HB3	6	0.28
(2,2238)	1:23:A:VAL:HG11	1:51:A:LEU:H	10	0.28
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	10	0.28
(2,2204)	1:20:A:GLU:HG3	1:19:A:ASP:H	6	0.28
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE1	5	0.28
(2,2073)	1:7:A:LEU:HD11	1:7:A:LEU:H	6	0.28
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG22	1	0.28
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	2	0.28
(2,2005)	2:164:B:SER:HA	2:164:B:SER:HB2	2	0.28
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG12	1	0.28
(2,1994)	2:161:B:LYS:HE3	2:161:B:LYS:HB2	7	0.28
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG3	6	0.28
(2,1962)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	5	0.28
(2,1944)	2:154:B:VAL:HG22	2:154:B:VAL:HA	7	0.28
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	10	0.28
(2,1885)	2:145:B:GLU:HA	2:145:B:GLU:HG2	1	0.28
(2,1881)	2:144:B:SER:HA	2:147:B:ASN:HB3	10	0.28
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	7	0.28
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB3	3	0.28
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	4	0.28
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	9	0.28
(2,1719)	2:121:B:LYS:HD3	2:121:B:LYS:HG2	6	0.28
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB3	7	0.28
(2,1613)	2:101:B:MET:HE3	2:101:B:MET:HG2	7	0.28
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	4	0.28
(2,1494)	1:41:A:PRO:HA	1:39:A:VAL:HG13	5	0.28
(2,1387)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	6	0.28
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	3	0.28
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	4	0.28
(2,1307)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	9	0.28
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG21	4	0.28
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG22	5	0.28
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG21	9	0.28
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	6	0.28
(2,1234)	2:163:B:ALA:HB1	2:163:B:ALA:HA	8	0.28
(2,1228)	2:162:B:LEU:HD12	2:162:B:LEU:HG	6	0.28
(2,1228)	2:162:B:LEU:HD23	2:162:B:LEU:HG	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1216)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	4	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	2	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	3	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	4	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	5	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	6	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	7	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	9	0.28
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.28
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	7	0.28
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	4	0.28
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB2	5	0.28
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB1	6	0.28
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	2	0.28
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	4	0.28
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	5	0.28
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	8	0.28
(2,1136)	2:104:B:VAL:HA	2:146:B:LEU:HD22	1	0.28
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	1	0.28
(2,1085)	2:142:B:VAL:HA	2:142:B:VAL:HG21	9	0.28
(2,1082)	2:142:B:VAL:HG11	2:103:B:TYR:HD2	6	0.28
(2,1081)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	4	0.28
(2,1034)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	8	0.28
(2,1028)	2:134:B:ALA:HB3	2:124:B:LYS:HA	9	0.28
(2,1028)	2:134:B:ALA:HB1	2:124:B:LYS:HA	10	0.28
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	6	0.28
(2,1023)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.28
(2,919)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	3	0.28
(2,919)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	5	0.28
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	6	0.28
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	2	0.28
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	10	0.28
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	7	0.28
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	10	0.28
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	7	0.28
(2,704)	1:54:A:VAL:HG22	1:58:A:SER:HB2	8	0.28
(2,695)	1:51:A:LEU:HD11	1:48:A:ALA:HA	1	0.28
(2,695)	1:51:A:LEU:HD11	1:48:A:ALA:HA	2	0.28
(2,695)	1:51:A:LEU:HD13	1:48:A:ALA:HA	3	0.28
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	3	0.28
(2,658)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	4	0.28
(2,657)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG13	4	0.28
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB3	8	0.28
(2,502)	1:26:A:ASP:HB2	1:30:A:ALA:HB3	6	0.28
(2,497)	1:25:A:GLU:HA	1:25:A:GLU:HG2	2	0.28
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG23	6	0.28
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	10	0.28
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	9	0.28
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	6	0.28
(2,389)	1:10:A:ILE:HD11	1:7:A:LEU:HG	2	0.28
(2,389)	1:10:A:ILE:HD11	1:7:A:LEU:HG	5	0.28
(2,389)	1:10:A:ILE:HD11	1:7:A:LEU:HG	7	0.28
(2,389)	1:10:A:ILE:HD12	1:7:A:LEU:HG	8	0.28
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	9	0.28
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	10	0.28
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB3	4	0.28
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	9	0.28
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	3	0.28
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG13	6	0.28
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB2	1	0.28
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	1	0.28
(2,207)	2:115:B:ASN:H	2:115:B:ASN:HD21	7	0.28
(2,182)	2:108:B:LEU:H	2:111:B:ALA:HB3	3	0.28
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD12	9	0.28
(2,4566)	2:165:B:VAL:H	2:165:B:VAL:HB	9	0.27
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	3	0.27
(2,4391)	1:61:A:CYS:HA	1:62:A:ASN:HA	3	0.27
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	2	0.27
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	10	0.27
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	8	0.27
(2,4090)	2:132:B:ILE:HA	2:132:B:ILE:HG12	2	0.27
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	4	0.27
(2,3509)	2:159:B:ILE:HG21	1:10:A:ILE:HG12	9	0.27
(2,3507)	2:159:B:ILE:HG23	1:60:A:ILE:HG13	2	0.27
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	7	0.27
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	4	0.27
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	10	0.27
(2,3495)	2:156:B:ALA:HB2	1:7:A:LEU:HD21	10	0.27
(2,3492)	2:152:B:GLU:HG2	1:7:A:LEU:HB3	8	0.27
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	5	0.27
(2,3410)	1:60:A:ILE:HD12	2:159:B:ILE:HG21	6	0.27
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	4	0.27
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	4	0.27
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	10	0.27
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	5	0.27
(2,3393)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	5	0.27
(2,3388)	1:37:A:VAL:HG11	2:109:B:LEU:HD11	2	0.27
(2,3307)	1:4:A:VAL:HG22	2:112:B:LEU:HA	3	0.27
(2,3298)	1:1:A:MET:HG3	2:153:B:ASP:HB2	9	0.27
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	3	0.27
(2,3261)	2:163:B:ALA:HB2	2:163:B:ALA:H	4	0.27
(2,3261)	2:163:B:ALA:HB3	2:163:B:ALA:H	7	0.27
(2,3260)	2:163:B:ALA:HB3	2:163:B:ALA:HA	2	0.27
(2,3253)	2:162:B:LEU:HD12	2:162:B:LEU:HG	5	0.27
(2,3253)	2:162:B:LEU:HD11	2:162:B:LEU:HG	7	0.27
(2,3253)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.27
(2,3247)	2:162:B:LEU:H	2:162:B:LEU:HB2	3	0.27
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	9	0.27
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG23	10	0.27
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	3	0.27
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	7	0.27
(2,3054)	2:142:B:VAL:HG11	2:107:B:TYR:HD2	2	0.27
(2,2888)	1:34:A:ALA:HB1	2:126:B:ILE:HD13	4	0.27
(2,2855)	2:124:B:LYS:HA	2:124:B:LYS:HE2	4	0.27
(2,2855)	2:124:B:LYS:HA	2:124:B:LYS:HE2	10	0.27
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	1	0.27
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	4	0.27
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	8	0.27
(2,2768)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	5	0.27
(2,2714)	2:110:B:ALA:HB3	2:123:B:ILE:H	5	0.27
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	6	0.27
(2,2558)	1:59:A:LEU:HD12	1:59:A:LEU:HG	1	0.27
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	7	0.27
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB2	3	0.27
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	10	0.27
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD13	8	0.27
(2,2388)	1:37:A:VAL:HG23	1:38:A:ASN:HB3	1	0.27
(2,2368)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	5	0.27
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	7	0.27
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	9	0.27
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	3	0.27
(2,2238)	1:23:A:VAL:HG12	1:51:A:LEU:H	7	0.27
(2,2209)	1:21:A:VAL:HG12	1:19:A:ASP:H	4	0.27
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG12	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG21	2	0.27
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG23	3	0.27
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG21	6	0.27
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG21	8	0.27
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG3	5	0.27
(2,1967)	2:157:B:GLN:HA	2:157:B:GLN:HG2	10	0.27
(2,1928)	2:151:B:ILE:HG21	2:151:B:ILE:HG13	4	0.27
(2,1885)	2:145:B:GLU:HA	2:145:B:GLU:HG2	2	0.27
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	2	0.27
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD3	3	0.27
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	2	0.27
(2,1712)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	7	0.27
(2,1712)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	10	0.27
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	10	0.27
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	1	0.27
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	8	0.27
(2,1678)	2:110:B:ALA:HB2	2:118:B:PRO:HA	4	0.27
(2,1629)	2:105:B:ALA:HB2	2:101:B:MET:HG2	5	0.27
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG2	9	0.27
(2,1614)	2:101:B:MET:HE1	1:14:A:LEU:HB2	2	0.27
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	2	0.27
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	5	0.27
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	10	0.27
(2,1540)	1:47:A:PHE:HA	1:51:A:LEU:HD13	5	0.27
(2,1532)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	2	0.27
(2,1418)	1:29:A:ASN:HA	1:29:A:ASN:HB3	4	0.27
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	10	0.27
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG22	1	0.27
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG23	7	0.27
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB2	10	0.27
(2,1234)	2:163:B:ALA:HB1	2:163:B:ALA:HA	7	0.27
(2,1228)	2:162:B:LEU:HD22	2:162:B:LEU:HG	3	0.27
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	2	0.27
(2,1205)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	1	0.27
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	10	0.27
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	1	0.27
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	4	0.27
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	4	0.27
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB3	10	0.27
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB3	2	0.27
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG22	2	0.27
(2,1070)	2:140:B:ASN:HA	2:143:B:ILE:HG23	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1034)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	9	0.27
(2,1023)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	7	0.27
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	8	0.27
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	1	0.27
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	3	0.27
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	5	0.27
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	7	0.27
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	8	0.27
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	9	0.27
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	1	0.27
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	4	0.27
(2,800)	2:105:B:ALA:HB3	2:101:B:MET:HG3	3	0.27
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	6	0.27
(2,787)	2:104:B:VAL:HA	2:146:B:LEU:HD21	3	0.27
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	3	0.27
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	3	0.27
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	8	0.27
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	10	0.27
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	6	0.27
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	5	0.27
(2,672)	1:49:A:LYS:HA	1:49:A:LYS:HB3	9	0.27
(2,658)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	6	0.27
(2,657)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	3	0.27
(2,657)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	10	0.27
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG11	7	0.27
(2,587)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	7	0.27
(2,558)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	2	0.27
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB3	8	0.27
(2,497)	1:25:A:GLU:HA	1:25:A:GLU:HG2	9	0.27
(2,439)	1:16:A:LEU:HD22	1:13:A:ALA:HA	2	0.27
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	2	0.27
(2,389)	1:10:A:ILE:HD12	1:7:A:LEU:HG	3	0.27
(2,389)	1:10:A:ILE:HD11	1:7:A:LEU:HG	4	0.27
(2,389)	1:10:A:ILE:HD12	1:7:A:LEU:HG	6	0.27
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	5	0.27
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	1	0.27
(2,327)	2:162:B:LEU:H	2:162:B:LEU:HB2	3	0.27
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG11	7	0.27
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	5	0.27
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	9	0.27
(2,213)	2:116:B:SER:H	2:117:B:SER:HB2	8	0.27
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB2	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG13	7	0.27
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	3	0.26
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	7	0.26
(2,4360)	1:52:A:ALA:HA	1:23:A:VAL:HG13	2	0.26
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	1	0.26
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	4	0.26
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	6	0.26
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	8	0.26
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	6	0.26
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	7	0.26
(2,4113)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	7	0.26
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	10	0.26
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	4	0.26
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	8	0.26
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	3	0.26
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	8	0.26
(2,3464)	2:129:B:SER:HA	1:34:A:ALA:HA	5	0.26
(2,3410)	1:60:A:ILE:HD12	2:159:B:ILE:HG21	10	0.26
(2,3402)	1:59:A:LEU:HD11	2:159:B:ILE:HA	2	0.26
(2,3399)	1:59:A:LEU:HD11	2:159:B:ILE:HA	2	0.26
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD23	2	0.26
(2,3331)	1:14:A:LEU:HD23	2:159:B:ILE:HA	6	0.26
(2,3301)	1:2:A:ALA:HB3	2:152:B:GLU:HA	10	0.26
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	4	0.26
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	10	0.26
(2,3261)	2:163:B:ALA:HB3	2:163:B:ALA:H	8	0.26
(2,3253)	2:162:B:LEU:HD11	2:162:B:LEU:HG	1	0.26
(2,3253)	2:162:B:LEU:HD11	2:162:B:LEU:HG	9	0.26
(2,3237)	2:161:B:LYS:HA	2:161:B:LYS:HG2	5	0.26
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG21	4	0.26
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG23	7	0.26
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG23	8	0.26
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG22	9	0.26
(2,3231)	2:159:B:ILE:HG23	2:159:B:ILE:H	3	0.26
(2,3195)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	6	0.26
(2,3090)	2:146:B:LEU:HA	2:146:B:LEU:HD22	2	0.26
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	1	0.26
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	4	0.26
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	7	0.26
(2,3062)	2:142:B:VAL:HG22	2:104:B:VAL:HA	8	0.26
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	7	0.26
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	1	0.26
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	1	0.26
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	3	0.26
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	5	0.26
(2,2842)	2:123:B:ILE:HG22	2:139:B:LEU:H	3	0.26
(2,2780)	2:116:B:SER:H	2:117:B:SER:HB3	6	0.26
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	9	0.26
(2,2777)	2:117:B:SER:HB2	2:118:B:PRO:HD3	10	0.26
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB3	8	0.26
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	5	0.26
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD21	9	0.26
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG11	2	0.26
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	2	0.26
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	2	0.26
(2,2527)	1:56:A:ILE:HD11	1:17:A:HIS:HD2	3	0.26
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD12	9	0.26
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	6	0.26
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	1	0.26
(2,2370)	1:38:A:ASN:H	1:37:A:VAL:HG21	7	0.26
(2,2269)	1:26:A:ASP:HB3	1:27:A:LYS:H	8	0.26
(2,2250)	1:25:A:GLU:HB3	1:28:A:ILE:H	6	0.26
(2,2209)	1:21:A:VAL:HG13	1:19:A:ASP:H	8	0.26
(2,2209)	1:21:A:VAL:HG13	1:19:A:ASP:H	9	0.26
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	6	0.26
(2,2098)	1:10:A:ILE:HD11	1:7:A:LEU:HG	9	0.26
(2,2048)	1:4:A:VAL:HB	1:4:A:VAL:HG23	10	0.26
(2,2015)	2:166:B:PRO:HG3	2:166:B:PRO:HA	7	0.26
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	3	0.26
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	2	0.26
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	4	0.26
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	9	0.26
(2,1856)	2:142:B:VAL:HA	2:142:B:VAL:HG21	9	0.26
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB3	8	0.26
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB3	2	0.26
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB2	8	0.26
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD2	7	0.26
(2,1742)	2:134:B:ALA:HB3	2:124:B:LYS:HA	6	0.26
(2,1712)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	8	0.26
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	3	0.26
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	8	0.26
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	7	0.26
(2,1678)	2:110:B:ALA:HB1	2:118:B:PRO:HA	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1672)	2:116:B:SER:HA	2:116:B:SER:HB3	5	0.26
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB2	6	0.26
(2,1333)	1:14:A:LEU:HD13	1:56:A:ILE:HG23	2	0.26
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG21	2	0.26
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG23	3	0.26
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG21	6	0.26
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG21	8	0.26
(2,1234)	2:163:B:ALA:HB1	2:163:B:ALA:HA	3	0.26
(2,1228)	2:162:B:LEU:HD11	2:162:B:LEU:HG	2	0.26
(2,1228)	2:162:B:LEU:HD12	2:162:B:LEU:HG	4	0.26
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	5	0.26
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	8	0.26
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	4	0.26
(2,1158)	2:151:B:ILE:HG21	2:151:B:ILE:HA	10	0.26
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	5	0.26
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	8	0.26
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	9	0.26
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	10	0.26
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD12	3	0.26
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB3	4	0.26
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD11	3	0.26
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD13	5	0.26
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD13	6	0.26
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	9	0.26
(2,846)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	4	0.26
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	5	0.26
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	8	0.26
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	6	0.26
(2,794)	2:104:B:VAL:HG11	2:105:B:ALA:HA	2	0.26
(2,792)	2:104:B:VAL:HG22	2:146:B:LEU:HD22	6	0.26
(2,761)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	0.26
(2,756)	1:65:A:ALA:HB1	1:65:A:ALA:HA	5	0.26
(2,695)	1:51:A:LEU:HD13	1:48:A:ALA:HA	5	0.26
(2,695)	1:51:A:LEU:HD11	1:48:A:ALA:HA	7	0.26
(2,682)	1:50:A:ALA:HB3	1:46:A:LEU:HB3	5	0.26
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	7	0.26
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	8	0.26
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	9	0.26
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	9	0.26
(2,493)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	1	0.26
(2,493)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	6	0.26
(2,488)	1:24:A:THR:HB	1:24:A:THR:HG23	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,422)	1:15:A:ILE:HD11	2:106:B:SER:HB2	5	0.26
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	4	0.26
(2,389)	1:10:A:ILE:HD12	1:7:A:LEU:HG	1	0.26
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	9	0.26
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	1	0.26
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG21	4	0.26
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG22	5	0.26
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG21	9	0.26
(2,335)	2:167:B:ALA:H	2:166:B:PRO:HB3	4	0.26
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	9	0.26
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	7	0.26
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB1	7	0.26
(2,253)	2:128:B:ASP:H	2:124:B:LYS:HD2	1	0.26
(2,253)	2:128:B:ASP:H	2:124:B:LYS:HD2	4	0.26
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD3	4	0.26
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	3	0.26
(2,201)	2:114:B:GLY:H	1:37:A:VAL:HG12	4	0.26
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	9	0.26
(2,128)	1:48:A:ALA:H	1:28:A:ILE:HD12	10	0.26
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	2	0.26
(2,4391)	1:61:A:CYS:HA	1:62:A:ASN:HA	1	0.25
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	1	0.25
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	3	0.25
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	5	0.25
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	8	0.25
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	9	0.25
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	10	0.25
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	9	0.25
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	7	0.25
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	1	0.25
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	2	0.25
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	5	0.25
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	7	0.25
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	8	0.25
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	1	0.25
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	3	0.25
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	7	0.25
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	6	0.25
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	2	0.25
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	5	0.25
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	6	0.25
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	8	0.25
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	4	0.25
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	8	0.25
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	8	0.25
(2,3401)	1:59:A:LEU:HD11	2:159:B:ILE:HG22	2	0.25
(2,3396)	1:39:A:VAL:HG23	2:112:B:LEU:HD22	7	0.25
(2,3388)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	5	0.25
(2,3303)	1:4:A:VAL:HG11	2:112:B:LEU:HD21	10	0.25
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	2	0.25
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	6	0.25
(2,3233)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	4	0.25
(2,3232)	2:159:B:ILE:HA	2:159:B:ILE:HG22	2	0.25
(2,3152)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	7	0.25
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	2	0.25
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	4	0.25
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	6	0.25
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	8	0.25
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	9	0.25
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	1	0.25
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	6	0.25
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	7	0.25
(2,3120)	2:147:B:ASN:HB3	2:148:B:GLY:H	8	0.25
(2,3109)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	5	0.25
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	5	0.25
(2,3055)	2:142:B:VAL:HA	2:142:B:VAL:HG21	8	0.25
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	3	0.25
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD13	6	0.25
(2,2871)	2:125:B:LYS:H	2:125:B:LYS:HD2	1	0.25
(2,2862)	2:124:B:LYS:HE3	2:124:B:LYS:HD2	6	0.25
(2,2855)	2:124:B:LYS:HA	2:124:B:LYS:HE3	3	0.25
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	3	0.25
(2,2723)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	6	0.25
(2,2646)	2:105:B:ALA:H	2:104:B:VAL:HG13	9	0.25
(2,2552)	1:59:A:LEU:HD22	1:59:A:LEU:HG	7	0.25
(2,2552)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.25
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	4	0.25
(2,2543)	1:58:A:SER:HB2	1:59:A:LEU:HG	5	0.25
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	5	0.25
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	8	0.25
(2,2482)	1:50:A:ALA:HB3	1:54:A:VAL:HG22	9	0.25
(2,2458)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	1	0.25
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2388)	1:37:A:VAL:HG21	1:38:A:ASN:HB3	6	0.25
(2,2368)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	6	0.25
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	6	0.25
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	1	0.25
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	2	0.25
(2,2209)	1:21:A:VAL:HG12	1:19:A:ASP:H	10	0.25
(2,2162)	1:16:A:LEU:HD23	1:13:A:ALA:HA	4	0.25
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	7	0.25
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD11	1	0.25
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	6	0.25
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	7	0.25
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG12	1	0.25
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG12	10	0.25
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	4	0.25
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	10	0.25
(2,1962)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	1	0.25
(2,1944)	2:154:B:VAL:HG22	2:154:B:VAL:HA	5	0.25
(2,1904)	2:146:B:LEU:HA	2:146:B:LEU:HD22	2	0.25
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	5	0.25
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB3	1	0.25
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB2	7	0.25
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB3	1	0.25
(2,1758)	2:126:B:ILE:HA	2:125:B:LYS:HD2	4	0.25
(2,1721)	2:122:B:ASP:HA	2:125:B:LYS:HG2	1	0.25
(2,1712)	2:121:B:LYS:HD2	2:121:B:LYS:HE2	3	0.25
(2,1614)	2:101:B:MET:HE1	1:14:A:LEU:HB2	10	0.25
(2,1610)	1:65:A:ALA:HB1	1:65:A:ALA:HA	5	0.25
(2,1520)	1:47:A:PHE:HA	1:51:A:LEU:HD13	8	0.25
(2,1418)	1:29:A:ASN:HA	1:29:A:ASN:HB3	8	0.25
(2,1399)	1:25:A:GLU:HB3	1:48:A:ALA:HB3	9	0.25
(2,1399)	1:25:A:GLU:HB3	1:48:A:ALA:HB1	10	0.25
(2,1391)	1:24:A:THR:HG21	1:27:A:LYS:HE3	3	0.25
(2,1288)	1:4:A:VAL:HB	1:4:A:VAL:HG23	10	0.25
(2,1266)	1:1:A:MET:HG2	2:152:B:GLU:HG3	3	0.25
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	8	0.25
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	9	0.25
(2,1229)	2:162:B:LEU:HD11	2:159:B:ILE:HA	9	0.25
(2,1228)	2:162:B:LEU:HD11	2:162:B:LEU:HG	1	0.25
(2,1228)	2:162:B:LEU:HD12	2:162:B:LEU:HG	5	0.25
(2,1228)	2:162:B:LEU:HD11	2:162:B:LEU:HG	7	0.25
(2,1228)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.25
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	1	0.25
(2,1186)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	6	0.25
(2,1185)	2:156:B:ALA:HA	2:156:B:ALA:HB3	8	0.25
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	1	0.25
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	2	0.25
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	3	0.25
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	6	0.25
(2,1156)	2:151:B:ILE:HG22	2:151:B:ILE:HB	7	0.25
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD12	9	0.25
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB3	2	0.25
(2,1112)	2:143:B:ILE:HG23	2:119:B:SER:HB3	8	0.25
(2,1082)	2:142:B:VAL:HG13	2:103:B:TYR:HD2	2	0.25
(2,1082)	2:142:B:VAL:HG12	2:103:B:TYR:HD2	3	0.25
(2,1082)	2:142:B:VAL:HG13	2:103:B:TYR:HD2	10	0.25
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD13	1	0.25
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD13	7	0.25
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	2	0.25
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	7	0.25
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	10	0.25
(2,842)	2:109:B:LEU:HD22	1:12:A:SER:HA	2	0.25
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	3	0.25
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	4	0.25
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	2	0.25
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	3	0.25
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	6	0.25
(2,792)	2:104:B:VAL:HG22	2:146:B:LEU:HD22	7	0.25
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	1	0.25
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	7	0.25
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	9	0.25
(2,740)	1:59:A:LEU:HD12	1:56:A:ILE:HA	2	0.25
(2,683)	1:50:A:ALA:HB1	1:54:A:VAL:HG22	5	0.25
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	5	0.25
(2,680)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	6	0.25
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	3	0.25
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	5	0.25
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	4	0.25
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	6	0.25
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG11	1	0.25
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG13	3	0.25
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG11	6	0.25
(2,596)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	5	0.25
(2,587)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,587)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	3	0.25
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG23	5	0.25
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	4	0.25
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	9	0.25
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	10	0.25
(2,389)	1:10:A:ILE:HD11	1:7:A:LEU:HG	10	0.25
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG22	1	0.25
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG23	7	0.25
(2,357)	1:4:A:VAL:HG11	2:112:B:LEU:HA	4	0.25
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	5	0.25
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	2	0.25
(2,332)	2:165:B:VAL:H	2:164:B:SER:HB2	3	0.25
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	10	0.25
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB1	3	0.25
(2,253)	2:128:B:ASP:H	2:124:B:LYS:HD2	7	0.25
(2,253)	2:128:B:ASP:H	2:124:B:LYS:HD2	9	0.25
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD13	6	0.25
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD2	5	0.25
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD3	6	0.25
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD3	7	0.25
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD3	8	0.25
(2,195)	2:113:B:GLY:H	2:112:B:LEU:HD23	1	0.25
(2,109)	1:39:A:VAL:H	1:38:A:ASN:HB3	9	0.25
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	9	0.25
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	5	0.25
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	6	0.25
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	7	0.25
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	5	0.24
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	4	0.24
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	9	0.24
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	10	0.24
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	1	0.24
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	4	0.24
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	7	0.24
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	2	0.24
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	4	0.24
(2,4373)	1:59:A:LEU:HB3	1:59:A:LEU:H	6	0.24
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	3	0.24
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	5	0.24
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	3	0.24
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	4	0.24
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4015)	1:14:A:LEU:HG	1:14:A:LEU:HA	9	0.24
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	6	0.24
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	9	0.24
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	10	0.24
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	3	0.24
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	1	0.24
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	3	0.24
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	8	0.24
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	10	0.24
(2,3377)	1:34:A:ALA:HB2	2:126:B:ILE:HB	4	0.24
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	4	0.24
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	10	0.24
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG13	1	0.24
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB2	4	0.24
(2,3203)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	3	0.24
(2,3178)	2:154:B:VAL:H	2:154:B:VAL:HG23	9	0.24
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	1	0.24
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	5	0.24
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	2	0.24
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	5	0.24
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	8	0.24
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	10	0.24
(2,3120)	2:147:B:ASN:HB3	2:148:B:GLY:H	3	0.24
(2,3120)	2:147:B:ASN:HB2	2:148:B:GLY:H	10	0.24
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG23	3	0.24
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	8	0.24
(2,3049)	2:142:B:VAL:HG12	2:107:B:TYR:HE2	6	0.24
(2,3018)	2:139:B:LEU:HD11	2:138:B:ARG:H	4	0.24
(2,3018)	2:139:B:LEU:HD13	2:138:B:ARG:H	5	0.24
(2,3018)	2:139:B:LEU:HD13	2:138:B:ARG:H	9	0.24
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	1	0.24
(2,2992)	2:137:B:ASP:HA	2:140:B:ASN:HB3	9	0.24
(2,2991)	2:137:B:ASP:HA	2:141:B:LYS:HB2	2	0.24
(2,2945)	2:132:B:ILE:HD12	2:133:B:GLU:H	3	0.24
(2,2945)	2:132:B:ILE:HD12	2:133:B:GLU:H	8	0.24
(2,2709)	2:109:B:LEU:HD22	1:12:A:SER:HA	2	0.24
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	10	0.24
(2,2589)	1:62:A:ASN:HB3	1:43:A:TRP:HZ2	7	0.24
(2,2552)	1:59:A:LEU:HD23	1:59:A:LEU:HG	2	0.24
(2,2552)	1:59:A:LEU:HD22	1:59:A:LEU:HG	3	0.24
(2,2552)	1:59:A:LEU:HD23	1:59:A:LEU:HG	5	0.24
(2,2552)	1:59:A:LEU:HD13	1:59:A:LEU:HG	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2540)	1:54:A:VAL:HG21	1:58:A:SER:HB3	4	0.24
(2,2527)	1:56:A:ILE:HD11	1:17:A:HIS:HD2	5	0.24
(2,2527)	1:56:A:ILE:HD13	1:17:A:HIS:HD2	7	0.24
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD11	1	0.24
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD13	4	0.24
(2,2405)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	9	0.24
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	4	0.24
(2,2238)	1:23:A:VAL:HG12	1:51:A:LEU:H	8	0.24
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	7	0.24
(2,2209)	1:21:A:VAL:HG13	1:19:A:ASP:H	6	0.24
(2,2142)	1:15:A:ILE:HD12	1:15:A:ILE:HA	1	0.24
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	4	0.24
(2,2098)	1:10:A:ILE:HD11	1:7:A:LEU:HG	5	0.24
(2,2098)	1:10:A:ILE:HD11	1:7:A:LEU:HG	7	0.24
(2,2098)	1:10:A:ILE:HD12	1:7:A:LEU:HG	8	0.24
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	1	0.24
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	2	0.24
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	7	0.24
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	8	0.24
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG11	10	0.24
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	4	0.24
(2,1967)	2:157:B:GLN:HA	2:157:B:GLN:HG2	7	0.24
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	4	0.24
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	9	0.24
(2,1829)	2:137:B:ASP:HA	2:141:B:LYS:HB2	2	0.24
(2,1792)	2:130:B:VAL:HG22	2:127:B:LEU:HA	3	0.24
(2,1712)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	5	0.24
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	6	0.24
(2,1680)	2:118:B:PRO:HA	2:118:B:PRO:HD3	3	0.24
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	9	0.24
(2,1629)	2:105:B:ALA:HB3	2:101:B:MET:HG2	10	0.24
(2,1613)	2:101:B:MET:HE2	2:101:B:MET:HG2	10	0.24
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	1	0.24
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	7	0.24
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	9	0.24
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB2	7	0.24
(2,1561)	1:56:A:ILE:HD13	1:10:A:ILE:HG21	5	0.24
(2,1381)	1:23:A:VAL:HG12	1:48:A:ALA:HB2	6	0.24
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	7	0.24
(2,1234)	2:163:B:ALA:HB3	2:163:B:ALA:HA	1	0.24
(2,1234)	2:163:B:ALA:HB3	2:163:B:ALA:HA	4	0.24
(2,1228)	2:162:B:LEU:HD11	2:162:B:LEU:HG	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	3	0.24
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	9	0.24
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	2	0.24
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD11	8	0.24
(2,1130)	2:146:B:LEU:HD22	2:146:B:LEU:HG	6	0.24
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB3	5	0.24
(2,1081)	2:142:B:VAL:HG12	2:107:B:TYR:HE2	6	0.24
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD13	9	0.24
(2,1041)	2:137:B:ASP:HA	2:141:B:LYS:HB2	2	0.24
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	1	0.24
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	3	0.24
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	8	0.24
(2,919)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	4	0.24
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	4	0.24
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	7	0.24
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	9	0.24
(2,875)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	6	0.24
(2,833)	2:109:B:LEU:HB3	2:110:B:ALA:HA	1	0.24
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	1	0.24
(2,796)	2:104:B:VAL:HA	2:104:B:VAL:HG13	5	0.24
(2,794)	2:104:B:VAL:HG21	2:105:B:ALA:HA	5	0.24
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	10	0.24
(2,775)	1:14:A:LEU:HD12	2:101:B:MET:HE1	3	0.24
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	3	0.24
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	4	0.24
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	10	0.24
(2,738)	1:59:A:LEU:HD22	1:59:A:LEU:HG	7	0.24
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG22	1	0.24
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG12	2	0.24
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG12	3	0.24
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG23	9	0.24
(2,683)	1:50:A:ALA:HB3	1:54:A:VAL:HG22	6	0.24
(2,682)	1:50:A:ALA:HB1	1:46:A:LEU:HB3	7	0.24
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	7	0.24
(2,660)	1:46:A:LEU:HD22	1:42:A:PHE:HD2	6	0.24
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	2	0.24
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG12	2	0.24
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG13	9	0.24
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG11	10	0.24
(2,596)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	6	0.24
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	1	0.24
(2,558)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG23	2	0.24
(2,434)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	1	0.24
(2,427)	1:15:A:ILE:HG22	2:127:B:LEU:HG	4	0.24
(2,426)	1:15:A:ILE:HG21	1:18:A:ASP:HB3	3	0.24
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE1	5	0.24
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	5	0.24
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	5	0.24
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG21	2	0.24
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG23	3	0.24
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG21	6	0.24
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG21	8	0.24
(2,332)	2:165:B:VAL:H	2:164:B:SER:HB3	1	0.24
(2,296)	2:144:B:SER:H	2:141:B:LYS:HG3	1	0.24
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	7	0.24
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	8	0.24
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD2	10	0.24
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	4	0.24
(2,162)	1:65:A:ALA:H	1:65:A:ALA:HB1	2	0.24
(2,161)	1:64:A:GLY:H	1:64:A:GLY:HA2	2	0.24
(2,66)	1:25:A:GLU:H	1:24:A:THR:HG21	4	0.24
(2,43)	1:16:A:LEU:H	1:16:A:LEU:HD12	4	0.24
(2,36)	1:13:A:ALA:H	1:59:A:LEU:HD11	3	0.24
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	3	0.24
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	8	0.24
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	3	0.24
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	7	0.24
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	7	0.23
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	7	0.23
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	6	0.23
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	5	0.23
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	7	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	1	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	2	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	3	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	4	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	5	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	6	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	7	0.23
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	10	0.23
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	3	0.23
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	7	0.23
(2,4002)	2:165:B:VAL:H	2:165:B:VAL:HB	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	4	0.23
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	6	0.23
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	2	0.23
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	10	0.23
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	7	0.23
(2,3509)	2:159:B:ILE:HG21	1:10:A:ILE:HG12	1	0.23
(2,3497)	1:59:A:LEU:HD12	2:159:B:ILE:HB	5	0.23
(2,3469)	2:130:B:VAL:HG21	1:16:A:LEU:HB2	8	0.23
(2,3454)	1:35:A:ALA:HB1	2:126:B:ILE:HD13	9	0.23
(2,3405)	1:59:A:LEU:HD12	2:159:B:ILE:HB	5	0.23
(2,3403)	1:59:A:LEU:HD12	2:159:B:ILE:HB	5	0.23
(2,3386)	1:37:A:VAL:HG12	2:109:B:LEU:HD13	10	0.23
(2,3378)	1:35:A:ALA:HB1	2:126:B:ILE:HD13	9	0.23
(2,3361)	1:31:A:LEU:HD12	2:129:B:SER:HA	10	0.23
(2,3334)	1:14:A:LEU:HD12	2:162:B:LEU:HD22	4	0.23
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG22	7	0.23
(2,3303)	1:4:A:VAL:HG22	2:112:B:LEU:HD11	2	0.23
(2,3301)	1:2:A:ALA:HB1	2:152:B:GLU:HA	9	0.23
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	2	0.23
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	6	0.23
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG11	2	0.23
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG13	8	0.23
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG12	10	0.23
(2,3267)	2:165:B:VAL:HA	2:165:B:VAL:HG22	9	0.23
(2,3231)	2:159:B:ILE:HG23	2:159:B:ILE:H	5	0.23
(2,3203)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	2	0.23
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	1	0.23
(2,3148)	2:151:B:ILE:HG21	2:151:B:ILE:HA	10	0.23
(2,3090)	2:146:B:LEU:HA	2:146:B:LEU:HD22	7	0.23
(2,3049)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	10	0.23
(2,3018)	2:139:B:LEU:HD13	2:138:B:ARG:H	1	0.23
(2,3018)	2:139:B:LEU:HD13	2:138:B:ARG:H	7	0.23
(2,3018)	2:139:B:LEU:HD13	2:138:B:ARG:H	10	0.23
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	3	0.23
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB1	2	0.23
(2,2921)	1:31:A:LEU:HD12	2:129:B:SER:HA	10	0.23
(2,2888)	1:34:A:ALA:HB1	2:126:B:ILE:HD12	5	0.23
(2,2871)	2:125:B:LYS:H	2:125:B:LYS:HD3	2	0.23
(2,2822)	2:120:B:ALA:HB3	2:140:B:ASN:H	6	0.23
(2,2742)	1:37:A:VAL:HG23	2:112:B:LEU:HD21	8	0.23
(2,2723)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	5	0.23
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	5	0.23
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	3	0.23
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	4	0.23
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	7	0.23
(2,2552)	1:59:A:LEU:HD12	1:59:A:LEU:HG	6	0.23
(2,2552)	1:59:A:LEU:HD13	1:59:A:LEU:HG	9	0.23
(2,2543)	1:58:A:SER:HB2	1:59:A:LEU:HG	3	0.23
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	8	0.23
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	10	0.23
(2,2368)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	4	0.23
(2,2368)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	9	0.23
(2,2318)	1:32:A:ILE:HD13	1:9:A:CYS:H	7	0.23
(2,2258)	1:25:A:GLU:HG2	1:48:A:ALA:HB3	5	0.23
(2,2250)	1:25:A:GLU:HB3	1:28:A:ILE:H	7	0.23
(2,2250)	1:25:A:GLU:HB3	1:28:A:ILE:H	8	0.23
(2,2209)	1:21:A:VAL:HG13	1:19:A:ASP:H	3	0.23
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	9	0.23
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE2	9	0.23
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	10	0.23
(2,2098)	1:10:A:ILE:HD11	1:7:A:LEU:HG	2	0.23
(2,2098)	1:10:A:ILE:HD12	1:7:A:LEU:HG	3	0.23
(2,2073)	1:7:A:LEU:HD11	1:7:A:LEU:H	4	0.23
(2,2034)	1:2:A:ALA:HB2	1:6:A:GLU:H	5	0.23
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	6	0.23
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	9	0.23
(2,1994)	2:161:B:LYS:HE3	2:161:B:LYS:HB2	1	0.23
(2,1988)	2:161:B:LYS:HD3	2:161:B:LYS:HA	3	0.23
(2,1946)	2:154:B:VAL:HG22	2:149:B:LYS:HG3	7	0.23
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG22	1	0.23
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	5	0.23
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	5	0.23
(2,1931)	2:152:B:GLU:HA	2:152:B:GLU:HB3	1	0.23
(2,1873)	2:143:B:ILE:HD12	2:142:B:VAL:HG13	7	0.23
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB3	2	0.23
(2,1742)	2:134:B:ALA:HB3	2:124:B:LYS:HA	7	0.23
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB2	9	0.23
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD3	8	0.23
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	2	0.23
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	3	0.23
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	4	0.23
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	10	0.23
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB3	1	0.23
(2,1540)	1:47:A:PHE:HA	1:51:A:LEU:HD12	10	0.23
(2,1536)	1:51:A:LEU:HD11	1:51:A:LEU:HG	5	0.23
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB2	6	0.23
(2,1450)	1:33:A:LYS:HG2	1:33:A:LYS:HD3	8	0.23
(2,1402)	1:26:A:ASP:HB3	1:26:A:ASP:HA	6	0.23
(2,1387)	1:23:A:VAL:HG11	1:48:A:ALA:HB2	8	0.23
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	6	0.23
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG21	5	0.23
(2,1307)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	1	0.23
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG13	1	0.23
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG13	8	0.23
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	8	0.23
(2,1234)	2:163:B:ALA:HB3	2:163:B:ALA:HA	5	0.23
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	5	0.23
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	9	0.23
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	4	0.23
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG21	9	0.23
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	8	0.23
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	9	0.23
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	9	0.23
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	6	0.23
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB2	1	0.23
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB2	4	0.23
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB3	6	0.23
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB3	7	0.23
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB2	8	0.23
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB2	9	0.23
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG22	3	0.23
(2,1081)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	10	0.23
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD11	2	0.23
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG3	1	0.23
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	2	0.23
(2,918)	2:121:B:LYS:HA	2:121:B:LYS:HB3	8	0.23
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	5	0.23
(2,829)	2:108:B:LEU:HD13	2:154:B:VAL:HB	9	0.23
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	7	0.23
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	7	0.23
(2,775)	1:14:A:LEU:HD12	2:101:B:MET:HE2	7	0.23
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	2	0.23
(2,740)	1:59:A:LEU:HD12	1:56:A:ILE:HA	1	0.23
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	10	0.23
(2,739)	1:59:A:LEU:HD13	1:56:A:ILE:HA	5	0.23
(2,738)	1:59:A:LEU:HD23	1:59:A:LEU:HG	2	0.23
(2,738)	1:59:A:LEU:HD22	1:59:A:LEU:HG	3	0.23
(2,738)	1:59:A:LEU:HD23	1:59:A:LEU:HG	5	0.23
(2,738)	1:59:A:LEU:HD23	1:59:A:LEU:HG	10	0.23
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	3	0.23
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	3	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG21	4	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG23	6	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG12	7	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG21	8	0.23
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG22	10	0.23
(2,680)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	2	0.23
(2,658)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	2	0.23
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD2	4	0.23
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	1	0.23
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	7	0.23
(2,620)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	3	0.23
(2,615)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	2	0.23
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG21	10	0.23
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	1	0.23
(2,439)	1:16:A:LEU:HD23	1:13:A:ALA:HA	6	0.23
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	3	0.23
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	7	0.23
(2,359)	1:4:A:VAL:HB	1:4:A:VAL:HG23	10	0.23
(2,334)	2:167:B:ALA:H	2:167:B:ALA:HB2	2	0.23
(2,322)	2:158:B:GLY:H	2:156:B:ALA:HB1	7	0.23
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	6	0.23
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB1	8	0.23
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	4	0.23
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	9	0.23
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB2	1	0.23
(2,211)	2:116:B:SER:H	2:115:B:ASN:HB2	3	0.23
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB1	2	0.23
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB1	8	0.23
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG13	1	0.23
(2,162)	1:65:A:ALA:H	1:65:A:ALA:HB3	8	0.23
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD13	8	0.23
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD12	9	0.23
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	1	0.23
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	8	0.23
(2,128)	1:48:A:ALA:H	1:28:A:ILE:HD12	7	0.23
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	6	0.23
(2,109)	1:39:A:VAL:H	1:38:A:ASN:HB3	6	0.23
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	1	0.23
(1,83)	2:139:B:LEU:N	2:135:B:ASP:O	4	0.23
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	5	0.23
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	6	0.23
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	9	0.23
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	5	0.22
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	6	0.22
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	5	0.22
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	4	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	1	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	2	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	3	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	4	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	6	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	8	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	9	0.22
(2,4164)	1:59:A:LEU:HB3	1:59:A:LEU:HG	10	0.22
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	8	0.22
(2,4149)	1:39:A:VAL:HA	1:39:A:VAL:HB	9	0.22
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	1	0.22
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	8	0.22
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	2	0.22
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	8	0.22
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	1	0.22
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	1	0.22
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	5	0.22
(2,3509)	2:159:B:ILE:HG21	1:10:A:ILE:HG12	2	0.22
(2,3509)	2:159:B:ILE:HG21	1:10:A:ILE:HG12	3	0.22
(2,3509)	2:159:B:ILE:HG21	1:10:A:ILE:HG12	5	0.22
(2,3509)	2:159:B:ILE:HG22	1:10:A:ILE:HG12	7	0.22
(2,3509)	2:159:B:ILE:HG22	1:10:A:ILE:HG12	10	0.22
(2,3492)	2:152:B:GLU:HG2	1:7:A:LEU:HB3	6	0.22
(2,3474)	2:130:B:VAL:HG13	1:27:A:LYS:HE2	3	0.22
(2,3410)	1:60:A:ILE:HD12	2:159:B:ILE:HG21	7	0.22
(2,3410)	1:60:A:ILE:HD12	2:159:B:ILE:HG21	8	0.22
(2,3400)	1:59:A:LEU:HD11	2:159:B:ILE:HG22	2	0.22
(2,3364)	1:31:A:LEU:HD12	2:130:B:VAL:HA	6	0.22
(2,3334)	1:14:A:LEU:HD11	2:162:B:LEU:HD22	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3332)	1:14:A:LEU:HD12	2:101:B:MET:HG3	3	0.22
(2,3317)	1:8:A:ALA:HB2	2:109:B:LEU:HG	5	0.22
(2,3317)	1:8:A:ALA:HB2	2:109:B:LEU:HG	8	0.22
(2,3307)	1:4:A:VAL:HG23	2:112:B:LEU:HA	2	0.22
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	6	0.22
(2,3261)	2:163:B:ALA:HB2	2:163:B:ALA:H	1	0.22
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	1	0.22
(2,3018)	2:139:B:LEU:HD11	2:138:B:ARG:H	2	0.22
(2,3018)	2:139:B:LEU:HD11	2:138:B:ARG:H	6	0.22
(2,3017)	2:139:B:LEU:HD12	2:120:B:ALA:HA	4	0.22
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	6	0.22
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	4	0.22
(2,2949)	2:132:B:ILE:HD11	2:132:B:ILE:H	2	0.22
(2,2935)	2:130:B:VAL:HG13	1:27:A:LYS:HE2	3	0.22
(2,2720)	2:110:B:ALA:H	2:110:B:ALA:HB2	2	0.22
(2,2628)	2:101:B:MET:HE3	2:103:B:TYR:HA	1	0.22
(2,2625)	2:101:B:MET:HE3	2:105:B:ALA:HB2	9	0.22
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	7	0.22
(2,2589)	1:62:A:ASN:HB3	1:43:A:TRP:HZ2	6	0.22
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	1	0.22
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	9	0.22
(2,2561)	1:59:A:LEU:HD12	1:56:A:ILE:HA	2	0.22
(2,2557)	1:59:A:LEU:HD12	1:56:A:ILE:HA	2	0.22
(2,2552)	1:59:A:LEU:HD13	1:59:A:LEU:HG	4	0.22
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	9	0.22
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD12	10	0.22
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG3	6	0.22
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	5	0.22
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	9	0.22
(2,2368)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	8	0.22
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	2	0.22
(2,2258)	1:25:A:GLU:HG3	1:48:A:ALA:HB1	6	0.22
(2,2239)	1:24:A:THR:H	1:23:A:VAL:HG12	2	0.22
(2,2162)	1:16:A:LEU:HD22	1:13:A:ALA:HA	2	0.22
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD12	6	0.22
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD13	7	0.22
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD13	8	0.22
(2,2142)	1:15:A:ILE:HD13	1:15:A:ILE:HA	10	0.22
(2,2130)	1:14:A:LEU:HD12	2:101:B:MET:HG3	8	0.22
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	5	0.22
(2,2100)	1:10:A:ILE:HG21	1:47:A:PHE:HE2	2	0.22
(2,2098)	1:10:A:ILE:HD12	1:7:A:LEU:HG	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2098)	1:10:A:ILE:HD11	1:7:A:LEU:HG	4	0.22
(2,2098)	1:10:A:ILE:HD12	1:7:A:LEU:HG	6	0.22
(2,2073)	1:7:A:LEU:HD12	1:7:A:LEU:H	2	0.22
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	3	0.22
(2,2014)	2:166:B:PRO:HA	2:166:B:PRO:HB3	5	0.22
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	1	0.22
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	2	0.22
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	10	0.22
(2,1988)	2:161:B:LYS:HD3	2:161:B:LYS:HA	2	0.22
(2,1988)	2:161:B:LYS:HD3	2:161:B:LYS:HA	8	0.22
(2,1967)	2:157:B:GLN:HA	2:157:B:GLN:HG2	2	0.22
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	7	0.22
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	3	0.22
(2,1936)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	7	0.22
(2,1904)	2:146:B:LEU:HA	2:146:B:LEU:HD22	7	0.22
(2,1857)	2:142:B:VAL:HA	2:142:B:VAL:HG21	9	0.22
(2,1843)	2:139:B:LEU:HD13	2:143:B:ILE:HD12	3	0.22
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB2	4	0.22
(2,1792)	2:130:B:VAL:HG22	2:127:B:LEU:HA	8	0.22
(2,1742)	2:134:B:ALA:HB1	2:124:B:LYS:HA	2	0.22
(2,1742)	2:134:B:ALA:HB1	2:124:B:LYS:HA	5	0.22
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	5	0.22
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	5	0.22
(2,1613)	2:101:B:MET:HE3	2:101:B:MET:HG2	4	0.22
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	2	0.22
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	4	0.22
(2,1574)	1:59:A:LEU:HA	1:62:A:ASN:HB3	3	0.22
(2,1536)	1:51:A:LEU:HD11	1:51:A:LEU:HG	3	0.22
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB2	7	0.22
(2,1465)	1:37:A:VAL:HG22	1:4:A:VAL:HG11	9	0.22
(2,1391)	1:24:A:THR:HG22	1:27:A:LYS:HE3	7	0.22
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	1	0.22
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	2	0.22
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	3	0.22
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	4	0.22
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	7	0.22
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	2	0.22
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	6	0.22
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	8	0.22
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG11	2	0.22
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG12	10	0.22
(2,1234)	2:163:B:ALA:HB3	2:163:B:ALA:HA	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1234)	2:163:B:ALA:HB3	2:163:B:ALA:HA	6	0.22
(2,1234)	2:163:B:ALA:HB3	2:163:B:ALA:HA	10	0.22
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	2	0.22
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	4	0.22
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	6	0.22
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	7	0.22
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	10	0.22
(2,1181)	2:155:B:ILE:HG21	2:155:B:ILE:HA	1	0.22
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	1	0.22
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	10	0.22
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	10	0.22
(2,1130)	2:146:B:LEU:HD11	2:146:B:LEU:HG	10	0.22
(2,1115)	2:144:B:SER:HA	2:147:B:ASN:HB2	3	0.22
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG23	1	0.22
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG23	2	0.22
(2,998)	2:130:B:VAL:HG13	1:27:A:LYS:HE2	3	0.22
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	9	0.22
(2,920)	2:122:B:ASP:HA	2:125:B:LYS:HG2	1	0.22
(2,875)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	5	0.22
(2,866)	2:112:B:LEU:HD12	2:108:B:LEU:HB2	6	0.22
(2,842)	2:109:B:LEU:HD23	1:12:A:SER:HA	5	0.22
(2,842)	2:109:B:LEU:HD21	1:12:A:SER:HA	7	0.22
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	2	0.22
(2,800)	2:105:B:ALA:HB3	2:101:B:MET:HG3	7	0.22
(2,774)	2:101:B:MET:HE3	2:103:B:TYR:HA	1	0.22
(2,756)	1:65:A:ALA:HB2	1:65:A:ALA:HA	6	0.22
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	4	0.22
(2,738)	1:59:A:LEU:HD12	1:59:A:LEU:HG	6	0.22
(2,738)	1:59:A:LEU:HD13	1:59:A:LEU:HG	8	0.22
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	2	0.22
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	4	0.22
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	5	0.22
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	2	0.22
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	4	0.22
(2,728)	1:54:A:VAL:HG23	1:58:A:SER:HB2	5	0.22
(2,709)	1:54:A:VAL:HB	1:54:A:VAL:HG23	5	0.22
(2,671)	1:49:A:LYS:HA	1:49:A:LYS:HD2	7	0.22
(2,658)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	8	0.22
(2,632)	1:42:A:PHE:HA	1:42:A:PHE:HD1	10	0.22
(2,622)	1:41:A:PRO:HA	1:39:A:VAL:HG13	5	0.22
(2,596)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	4	0.22
(2,596)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	6	0.22
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG3	10	0.22
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG23	4	0.22
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG13	3	0.22
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG21	5	0.22
(2,426)	1:15:A:ILE:HG21	1:18:A:ASP:HB3	5	0.22
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	2	0.22
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	3	0.22
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	7	0.22
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	8	0.22
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	8	0.22
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	1	0.22
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	2	0.22
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	4	0.22
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB1	6	0.22
(2,162)	1:65:A:ALA:H	1:65:A:ALA:HB1	1	0.22
(2,162)	1:65:A:ALA:H	1:65:A:ALA:HB1	6	0.22
(2,161)	1:64:A:GLY:H	1:64:A:GLY:HA3	7	0.22
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD23	10	0.22
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	10	0.22
(2,109)	1:39:A:VAL:H	1:38:A:ASN:HB3	5	0.22
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	4	0.22
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	5	0.22
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	6	0.21
(2,4538)	2:152:B:GLU:H	2:152:B:GLU:HG2	6	0.21
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	6	0.21
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	1	0.21
(2,4517)	2:144:B:SER:HA	2:143:B:ILE:HB	3	0.21
(2,4456)	2:124:B:LYS:HA	2:124:B:LYS:HD2	6	0.21
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	1	0.21
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	1	0.21
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	6	0.21
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	8	0.21
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	9	0.21
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	5	0.21
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	9	0.21
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	4	0.21
(2,3509)	2:159:B:ILE:HG22	1:10:A:ILE:HG12	8	0.21
(2,3488)	2:152:B:GLU:HB3	1:4:A:VAL:HG21	10	0.21
(2,3419)	2:105:B:ALA:HA	1:14:A:LEU:HD22	9	0.21
(2,3329)	1:11:A:TYR:HB2	2:109:B:LEU:HG	1	0.21
(2,3322)	1:10:A:ILE:HD11	2:159:B:ILE:HG22	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG21	9	0.21
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	4	0.21
(2,3317)	1:8:A:ALA:HB2	2:109:B:LEU:HG	7	0.21
(2,3307)	1:4:A:VAL:HG23	2:112:B:LEU:HA	8	0.21
(2,3303)	1:4:A:VAL:HG12	2:112:B:LEU:HD23	4	0.21
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB2	10	0.21
(2,3248)	2:162:B:LEU:HB3	2:162:B:LEU:HD21	8	0.21
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	3	0.21
(2,3205)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	1	0.21
(2,3151)	2:152:B:GLU:HB3	1:4:A:VAL:HG23	5	0.21
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	4	0.21
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	9	0.21
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	3	0.21
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	9	0.21
(2,3090)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.21
(2,3090)	2:146:B:LEU:HA	2:146:B:LEU:HD22	8	0.21
(2,3090)	2:146:B:LEU:HA	2:146:B:LEU:HD22	9	0.21
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	4	0.21
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	5	0.21
(2,3049)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	2	0.21
(2,3016)	2:139:B:LEU:HD12	2:140:B:ASN:HA	8	0.21
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	5	0.21
(2,2982)	2:134:B:ALA:HB1	2:124:B:LYS:HA	1	0.21
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB3	6	0.21
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB3	7	0.21
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB3	8	0.21
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB3	9	0.21
(2,2969)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	2	0.21
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD12	1	0.21
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD12	2	0.21
(2,2872)	2:125:B:LYS:HD2	2:125:B:LYS:HB3	4	0.21
(2,2861)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	4	0.21
(2,2850)	2:123:B:ILE:HG23	2:139:B:LEU:HA	6	0.21
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	4	0.21
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	3	0.21
(2,2720)	2:110:B:ALA:H	2:110:B:ALA:HB2	8	0.21
(2,2714)	2:110:B:ALA:HB3	2:123:B:ILE:H	8	0.21
(2,2709)	2:109:B:LEU:HD23	1:12:A:SER:HA	5	0.21
(2,2709)	2:109:B:LEU:HD23	1:12:A:SER:HA	6	0.21
(2,2709)	2:109:B:LEU:HD21	1:12:A:SER:HA	7	0.21
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	8	0.21
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG11	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG11	3	0.21
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG11	7	0.21
(2,2589)	1:62:A:ASN:HB2	1:43:A:TRP:HZ2	3	0.21
(2,2589)	1:62:A:ASN:HB3	1:43:A:TRP:HZ2	10	0.21
(2,2588)	1:63:A:VAL:H	1:62:A:ASN:HB2	2	0.21
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	8	0.21
(2,2561)	1:59:A:LEU:HD13	1:56:A:ILE:HA	10	0.21
(2,2557)	1:59:A:LEU:HD13	1:56:A:ILE:HA	10	0.21
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	3	0.21
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	4	0.21
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	6	0.21
(2,2496)	1:51:A:LEU:HB3	1:51:A:LEU:HD21	8	0.21
(2,2482)	1:50:A:ALA:HB1	1:54:A:VAL:HG12	4	0.21
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB2	6	0.21
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB2	7	0.21
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG3	4	0.21
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	4	0.21
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	10	0.21
(2,2364)	1:37:A:VAL:HA	1:38:A:ASN:HB2	8	0.21
(2,2346)	1:34:A:ALA:HB2	2:126:B:ILE:HG22	10	0.21
(2,2318)	1:32:A:ILE:HD13	1:9:A:CYS:H	8	0.21
(2,2261)	1:25:A:GLU:HG2	1:26:A:ASP:H	6	0.21
(2,2258)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	2	0.21
(2,2255)	1:25:A:GLU:HG2	1:26:A:ASP:HA	4	0.21
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	4	0.21
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	4	0.21
(2,2209)	1:21:A:VAL:HG13	1:19:A:ASP:H	5	0.21
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE2	4	0.21
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	3	0.21
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	7	0.21
(2,2098)	1:10:A:ILE:HD11	1:7:A:LEU:HG	10	0.21
(2,2073)	1:7:A:LEU:HD12	1:7:A:LEU:H	3	0.21
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG11	2	0.21
(2,2034)	1:2:A:ALA:HB2	1:6:A:GLU:H	1	0.21
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB2	4	0.21
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	8	0.21
(2,1988)	2:161:B:LYS:HD3	2:161:B:LYS:HA	1	0.21
(2,1962)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	3	0.21
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	7	0.21
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	8	0.21
(2,1834)	2:138:B:ARG:HG2	2:138:B:ARG:HD3	6	0.21
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB2	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB3	3	0.21
(2,1743)	2:124:B:LYS:HG2	2:124:B:LYS:HE3	5	0.21
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	7	0.21
(2,1712)	2:121:B:LYS:HD3	2:121:B:LYS:HE2	4	0.21
(2,1681)	2:118:B:PRO:HA	2:122:B:ASP:HB2	1	0.21
(2,1678)	2:110:B:ALA:HB1	2:118:B:PRO:HA	2	0.21
(2,1613)	2:101:B:MET:HE3	2:101:B:MET:HG2	9	0.21
(2,1610)	1:65:A:ALA:HB2	1:65:A:ALA:HA	6	0.21
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	3	0.21
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	7	0.21
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	8	0.21
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	9	0.21
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB2	10	0.21
(2,1561)	1:56:A:ILE:HD13	1:10:A:ILE:HG21	3	0.21
(2,1561)	1:56:A:ILE:HD12	1:10:A:ILE:HG21	10	0.21
(2,1536)	1:51:A:LEU:HD12	1:51:A:LEU:HG	1	0.21
(2,1536)	1:51:A:LEU:HD12	1:51:A:LEU:HG	2	0.21
(2,1536)	1:51:A:LEU:HD11	1:51:A:LEU:HG	4	0.21
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	2	0.21
(2,1465)	1:37:A:VAL:HG22	1:4:A:VAL:HG11	3	0.21
(2,1450)	1:33:A:LYS:HG2	1:33:A:LYS:HD3	2	0.21
(2,1450)	1:33:A:LYS:HG2	1:33:A:LYS:HD3	6	0.21
(2,1450)	1:33:A:LYS:HG3	1:33:A:LYS:HD2	9	0.21
(2,1450)	1:33:A:LYS:HG3	1:33:A:LYS:HD2	10	0.21
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	8	0.21
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG23	10	0.21
(2,1373)	1:22:A:THR:HG23	1:21:A:VAL:HB	5	0.21
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG23	2	0.21
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	1	0.21
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	3	0.21
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	3	0.21
(2,1230)	2:162:B:LEU:HD23	2:162:B:LEU:HG	8	0.21
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	1	0.21
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	2	0.21
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	10	0.21
(2,1218)	2:159:B:ILE:HG13	2:159:B:ILE:HG23	4	0.21
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG22	3	0.21
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG22	5	0.21
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG23	6	0.21
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	1	0.21
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	3	0.21
(2,1206)	2:159:B:ILE:HB	2:159:B:ILE:HD13	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	7	0.21
(2,1179)	2:155:B:ILE:HG21	2:155:B:ILE:HB	6	0.21
(2,1179)	2:155:B:ILE:HG21	2:155:B:ILE:HB	7	0.21
(2,1179)	2:155:B:ILE:HG23	2:155:B:ILE:HB	9	0.21
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD12	5	0.21
(2,1130)	2:146:B:LEU:HD22	2:146:B:LEU:HG	1	0.21
(2,1130)	2:146:B:LEU:HD22	2:146:B:LEU:HG	3	0.21
(2,1130)	2:146:B:LEU:HD12	2:146:B:LEU:HG	8	0.21
(2,1125)	2:146:B:LEU:HD22	2:145:B:GLU:HB2	3	0.21
(2,1114)	2:144:B:SER:HA	2:144:B:SER:HB2	3	0.21
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG22	8	0.21
(2,1085)	2:142:B:VAL:HA	2:142:B:VAL:HG21	8	0.21
(2,1081)	2:142:B:VAL:HG11	2:107:B:TYR:HE2	2	0.21
(2,1034)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	5	0.21
(2,1028)	2:134:B:ALA:HB1	2:124:B:LYS:HA	1	0.21
(2,842)	2:109:B:LEU:HD23	1:12:A:SER:HA	6	0.21
(2,842)	2:109:B:LEU:HD22	1:12:A:SER:HA	10	0.21
(2,836)	1:8:A:ALA:HA	2:109:B:LEU:HD13	5	0.21
(2,800)	2:105:B:ALA:HB3	2:101:B:MET:HG2	2	0.21
(2,800)	2:105:B:ALA:HB2	2:101:B:MET:HG3	8	0.21
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	1	0.21
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	9	0.21
(2,738)	1:59:A:LEU:HD13	1:59:A:LEU:HG	4	0.21
(2,738)	1:59:A:LEU:HD13	1:59:A:LEU:HG	9	0.21
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	1	0.21
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	6	0.21
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	8	0.21
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.21
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	1	0.21
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	5	0.21
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	6	0.21
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	8	0.21
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.21
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	2	0.21
(2,711)	1:55:A:ASN:HA	1:54:A:VAL:HG21	2	0.21
(2,707)	1:54:A:VAL:HG23	1:58:A:SER:HB2	5	0.21
(2,704)	1:54:A:VAL:HG22	1:58:A:SER:HB3	1	0.21
(2,695)	1:51:A:LEU:HD13	1:48:A:ALA:HA	4	0.21
(2,695)	1:51:A:LEU:HD13	1:48:A:ALA:HA	8	0.21
(2,683)	1:50:A:ALA:HB1	1:54:A:VAL:HG21	3	0.21
(2,682)	1:50:A:ALA:HB2	1:46:A:LEU:HB2	2	0.21
(2,673)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,658)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	1	0.21
(2,658)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	5	0.21
(2,658)	1:46:A:LEU:HD23	1:42:A:PHE:HZ	7	0.21
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD2	6	0.21
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	1	0.21
(2,596)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	8	0.21
(2,567)	1:34:A:ALA:HB2	2:126:B:ILE:HG22	10	0.21
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG2	1	0.21
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG3	5	0.21
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG2	7	0.21
(2,496)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	2	0.21
(2,496)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	3	0.21
(2,496)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	8	0.21
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG21	3	0.21
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG13	5	0.21
(2,434)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	4	0.21
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	2	0.21
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	10	0.21
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	8	0.21
(2,314)	2:153:B:ASP:H	2:154:B:VAL:HG21	6	0.21
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	1	0.21
(2,287)	2:141:B:LYS:H	2:142:B:VAL:HG11	3	0.21
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	8	0.21
(2,273)	2:136:B:ASP:H	2:139:B:LEU:HD11	2	0.21
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD12	1	0.21
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD12	2	0.21
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	6	0.21
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	7	0.21
(2,159)	1:63:A:VAL:H	1:62:A:ASN:HB2	5	0.21
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD23	2	0.21
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD23	5	0.21
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD23	6	0.21
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD22	7	0.21
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD22	8	0.21
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	4	0.21
(2,12)	1:3:A:SER:H	1:6:A:GLU:HG2	8	0.21
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	9	0.21
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	10	0.21
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	4	0.21
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	8	0.21
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	9	0.2
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	9	0.2
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	3	0.2
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	6	0.2
(2,4393)	1:63:A:VAL:HA	1:64:A:GLY:H	5	0.2
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	5	0.2
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	10	0.2
(2,4251)	1:15:A:ILE:HA	2:103:B:TYR:HA	3	0.2
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	5	0.2
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	6	0.2
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	4	0.2
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	10	0.2
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	1	0.2
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	5	0.2
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	8	0.2
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	3	0.2
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	1	0.2
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	8	0.2
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	8	0.2
(2,3596)	1:21:A:VAL:H	1:22:A:THR:H	9	0.2
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	8	0.2
(2,3493)	2:152:B:GLU:HG2	1:4:A:VAL:HB	8	0.2
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	3	0.2
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	6	0.2
(2,3393)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	4	0.2
(2,3393)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	6	0.2
(2,3387)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	7	0.2
(2,3322)	1:10:A:ILE:HD13	2:159:B:ILE:HG21	5	0.2
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	6	0.2
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	8	0.2
(2,3284)	2:166:B:PRO:HD3	2:166:B:PRO:HA	7	0.2
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG11	6	0.2
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD13	1	0.2
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD13	7	0.2
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD11	10	0.2
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	5	0.2
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	9	0.2
(2,3239)	2:161:B:LYS:HD3	2:161:B:LYS:HA	3	0.2
(2,3203)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	9	0.2
(2,3156)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	6	0.2
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	1	0.2
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	2	0.2
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	5	0.2
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	6	0.2
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	8	0.2
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	10	0.2
(2,3138)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	4	0.2
(2,3120)	2:147:B:ASN:HB3	2:148:B:GLY:H	4	0.2
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD22	4	0.2
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	10	0.2
(2,3049)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	9	0.2
(2,2992)	2:137:B:ASP:HA	2:140:B:ASN:HB3	2	0.2
(2,2985)	2:136:B:ASP:H	2:135:B:ASP:HB2	6	0.2
(2,2970)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	2	0.2
(2,2969)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	4	0.2
(2,2871)	2:125:B:LYS:H	2:125:B:LYS:HD2	3	0.2
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	7	0.2
(2,2765)	2:110:B:ALA:HB2	2:115:B:ASN:HB3	8	0.2
(2,2715)	2:110:B:ALA:HB2	2:115:B:ASN:H	1	0.2
(2,2715)	2:110:B:ALA:HB2	2:115:B:ASN:H	3	0.2
(2,2709)	2:109:B:LEU:HD22	1:12:A:SER:HA	3	0.2
(2,2709)	2:109:B:LEU:HD22	1:12:A:SER:HA	10	0.2
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	6	0.2
(2,2628)	2:101:B:MET:HE3	2:103:B:TYR:HA	4	0.2
(2,2625)	2:101:B:MET:HE3	2:105:B:ALA:HB2	4	0.2
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG11	1	0.2
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG12	8	0.2
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG12	9	0.2
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	7	0.2
(2,2561)	1:59:A:LEU:HD12	1:56:A:ILE:HA	1	0.2
(2,2561)	1:59:A:LEU:HD13	1:56:A:ILE:HA	8	0.2
(2,2557)	1:59:A:LEU:HD12	1:56:A:ILE:HA	1	0.2
(2,2557)	1:59:A:LEU:HD13	1:56:A:ILE:HA	8	0.2
(2,2552)	1:59:A:LEU:HD12	1:59:A:LEU:HG	1	0.2
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	3	0.2
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	1	0.2
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	2	0.2
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	5	0.2
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.2
(2,2543)	1:58:A:SER:HB2	1:59:A:LEU:HG	8	0.2
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	10	0.2
(2,2527)	1:56:A:ILE:HD13	1:17:A:HIS:HD2	10	0.2
(2,2458)	1:46:A:LEU:HD22	1:42:A:PHE:HD2	6	0.2
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	7	0.2
(2,2388)	1:37:A:VAL:HG23	1:38:A:ASN:HB3	3	0.2
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	2	0.2
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	7	0.2
(2,2368)	1:37:A:VAL:HG13	2:113:B:GLY:HA2	2	0.2
(2,2324)	1:32:A:ILE:HD12	1:31:A:LEU:H	2	0.2
(2,2324)	1:32:A:ILE:HD13	1:31:A:LEU:H	3	0.2
(2,2250)	1:25:A:GLU:HB3	1:28:A:ILE:H	3	0.2
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG23	9	0.2
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD12	9	0.2
(2,2142)	1:15:A:ILE:HD12	1:15:A:ILE:HA	9	0.2
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE2	3	0.2
(2,2073)	1:7:A:LEU:HD11	1:7:A:LEU:H	10	0.2
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG13	6	0.2
(2,2037)	1:3:A:SER:H	1:2:A:ALA:HB2	10	0.2
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	7	0.2
(2,1904)	2:146:B:LEU:HA	2:146:B:LEU:HD22	5	0.2
(2,1904)	2:146:B:LEU:HA	2:146:B:LEU:HD22	8	0.2
(2,1904)	2:146:B:LEU:HA	2:146:B:LEU:HD22	9	0.2
(2,1866)	2:143:B:ILE:HA	2:143:B:ILE:HG12	2	0.2
(2,1866)	2:143:B:ILE:HA	2:143:B:ILE:HG12	5	0.2
(2,1866)	2:143:B:ILE:HA	2:143:B:ILE:HG12	6	0.2
(2,1866)	2:143:B:ILE:HA	2:143:B:ILE:HG12	9	0.2
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB2	5	0.2
(2,1814)	2:133:B:GLU:HA	2:133:B:GLU:HG2	3	0.2
(2,1721)	2:122:B:ASP:HA	2:125:B:LYS:HG2	2	0.2
(2,1718)	2:121:B:LYS:HB2	2:121:B:LYS:HG2	4	0.2
(2,1561)	1:56:A:ILE:HD12	1:10:A:ILE:HG21	7	0.2
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	2	0.2
(2,1485)	1:39:A:VAL:HG13	1:43:A:TRP:HA	9	0.2
(2,1450)	1:33:A:LYS:HG2	1:33:A:LYS:HD3	3	0.2
(2,1450)	1:33:A:LYS:HG3	1:33:A:LYS:HD2	5	0.2
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG2	1	0.2
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG3	10	0.2
(2,1418)	1:29:A:ASN:HA	1:29:A:ASN:HB3	9	0.2
(2,1391)	1:24:A:THR:HG22	1:27:A:LYS:HE3	1	0.2
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG22	5	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG22	1	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG23	3	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG21	6	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG22	7	0.2
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG23	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG23	10	0.2
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	9	0.2
(2,1238)	2:165:B:VAL:HA	2:165:B:VAL:HG22	9	0.2
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	5	0.2
(2,1230)	2:162:B:LEU:HD12	2:162:B:LEU:HG	6	0.2
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	8	0.2
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG22	1	0.2
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	1	0.2
(2,1179)	2:155:B:ILE:HG21	2:155:B:ILE:HB	2	0.2
(2,1179)	2:155:B:ILE:HG22	2:155:B:ILE:HB	5	0.2
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	1	0.2
(2,1154)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	6	0.2
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	2	0.2
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	5	0.2
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	6	0.2
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	8	0.2
(2,1130)	2:146:B:LEU:HD11	2:146:B:LEU:HG	2	0.2
(2,1130)	2:146:B:LEU:HD13	2:146:B:LEU:HG	9	0.2
(2,1115)	2:144:B:SER:HA	2:147:B:ASN:HB2	1	0.2
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG22	5	0.2
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG22	9	0.2
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG23	10	0.2
(2,1081)	2:142:B:VAL:HG13	2:107:B:TYR:HE2	9	0.2
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD11	6	0.2
(2,1053)	2:139:B:LEU:HA	2:139:B:LEU:HD13	4	0.2
(2,956)	2:125:B:LYS:HA	2:125:B:LYS:HG3	1	0.2
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	10	0.2
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	2	0.2
(2,851)	2:107:B:TYR:HA	2:110:B:ALA:HB2	4	0.2
(2,842)	2:109:B:LEU:HD22	1:12:A:SER:HA	3	0.2
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	8	0.2
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	9	0.2
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	8	0.2
(2,774)	2:101:B:MET:HE3	2:103:B:TYR:HA	4	0.2
(2,752)	1:61:A:CYS:HB2	1:60:A:ILE:HG21	9	0.2
(2,735)	1:59:A:LEU:HA	1:59:A:LEU:HD21	5	0.2
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	7	0.2
(2,734)	1:59:A:LEU:HB2	1:56:A:ILE:HA	9	0.2
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	7	0.2
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	4	0.2
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	7	0.2
(2,719)	1:56:A:ILE:HD12	1:17:A:HIS:HD2	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG13	4	0.2
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG12	9	0.2
(2,683)	1:50:A:ALA:HB1	1:54:A:VAL:HG21	10	0.2
(2,671)	1:49:A:LYS:HA	1:49:A:LYS:HD2	6	0.2
(2,660)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	7	0.2
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	1	0.2
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	8	0.2
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	8	0.2
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	2	0.2
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	7	0.2
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG23	6	0.2
(2,496)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	5	0.2
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG22	7	0.2
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG22	8	0.2
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG21	5	0.2
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG13	6	0.2
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG12	10	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG22	1	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG23	2	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG23	3	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG21	6	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG23	8	0.2
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG23	10	0.2
(2,392)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	2	0.2
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	3	0.2
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	7	0.2
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	8	0.2
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	9	0.2
(2,357)	1:4:A:VAL:HG11	2:112:B:LEU:HA	5	0.2
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD22	1	0.2
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB2	9	0.2
(2,332)	2:165:B:VAL:H	2:164:B:SER:HB2	7	0.2
(2,324)	2:161:B:LYS:H	2:161:B:LYS:HG3	2	0.2
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	7	0.2
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	1	0.2
(2,279)	2:139:B:LEU:H	2:139:B:LEU:HD13	2	0.2
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	10	0.2
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	1	0.2
(2,200)	2:114:B:GLY:H	2:111:B:ALA:HB1	5	0.2
(2,199)	2:114:B:GLY:H	2:112:B:LEU:H	3	0.2
(2,195)	2:113:B:GLY:H	2:112:B:LEU:HD22	3	0.2
(2,169)	1:43:A:TRP:HE1	1:5:A:SER:HB2	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,169)	1:43:A:TRP:HE1	1:5:A:SER:HB2	9	0.2
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG12	3	0.2
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD22	3	0.2
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD23	4	0.2
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD23	9	0.2
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD11	1	0.2
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD13	4	0.2
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	3	0.2
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	4	0.2
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	2	0.2
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	5	0.2
(2,31)	1:12:A:SER:H	2:109:B:LEU:HD12	6	0.2
(2,20)	1:8:A:ALA:H	1:7:A:LEU:HD22	1	0.2
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	1	0.2
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	3	0.19
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	9	0.19
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	2	0.19
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	4	0.19
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	7	0.19
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	8	0.19
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	9	0.19
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	3	0.19
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	8	0.19
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	4	0.19
(2,4183)	2:125:B:LYS:HA	2:125:B:LYS:HB3	3	0.19
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	5	0.19
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	7	0.19
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	10	0.19
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	2	0.19
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	1	0.19
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	2	0.19
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	3	0.19
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	2	0.19
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	9	0.19
(2,3769)	2:106:B:SER:H	2:104:B:VAL:HB	5	0.19
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	1	0.19
(2,3509)	2:159:B:ILE:HG22	1:10:A:ILE:HG12	6	0.19
(2,3489)	2:152:B:GLU:HG3	1:7:A:LEU:HG	9	0.19
(2,3454)	1:35:A:ALA:HB1	2:126:B:ILE:HD12	6	0.19
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	4	0.19
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	5	0.19
(2,3378)	1:35:A:ALA:HB1	2:126:B:ILE:HD12	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3364)	1:31:A:LEU:HD21	2:130:B:VAL:HA	10	0.19
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	9	0.19
(2,3317)	1:8:A:ALA:HB2	2:109:B:LEU:HG	6	0.19
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	7	0.19
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	9	0.19
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD12	4	0.19
(2,3248)	2:162:B:LEU:HB3	2:162:B:LEU:HD21	6	0.19
(2,3239)	2:161:B:LYS:HD3	2:161:B:LYS:HA	2	0.19
(2,3239)	2:161:B:LYS:HD3	2:161:B:LYS:HA	8	0.19
(2,3184)	2:155:B:ILE:HG22	2:159:B:ILE:HG13	1	0.19
(2,3178)	2:154:B:VAL:H	2:154:B:VAL:HG23	3	0.19
(2,3144)	2:151:B:ILE:HG22	2:151:B:ILE:HB	7	0.19
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB3	10	0.19
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB3	2	0.19
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	10	0.19
(2,3018)	2:139:B:LEU:HD11	2:138:B:ARG:H	3	0.19
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	4	0.19
(2,3004)	2:138:B:ARG:HB3	2:138:B:ARG:HD2	3	0.19
(2,2976)	2:134:B:ALA:HB3	2:135:B:ASP:HB2	10	0.19
(2,2970)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	4	0.19
(2,2950)	2:132:B:ILE:HD13	2:130:B:VAL:H	8	0.19
(2,2949)	2:132:B:ILE:HD11	2:132:B:ILE:H	3	0.19
(2,2945)	2:132:B:ILE:HD13	2:133:B:GLU:H	5	0.19
(2,2822)	2:120:B:ALA:HB3	2:140:B:ASN:H	1	0.19
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	8	0.19
(2,2808)	2:119:B:SER:HB3	2:121:B:LYS:HD3	8	0.19
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	6	0.19
(2,2742)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	4	0.19
(2,2720)	2:110:B:ALA:H	2:110:B:ALA:HB2	5	0.19
(2,2720)	2:110:B:ALA:H	2:110:B:ALA:HB2	6	0.19
(2,2626)	2:101:B:MET:HE2	2:102:B:ARG:H	6	0.19
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG13	4	0.19
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG11	6	0.19
(2,2589)	1:62:A:ASN:HB2	1:43:A:TRP:HZ2	8	0.19
(2,2584)	1:61:A:CYS:HB3	1:62:A:ASN:HA	10	0.19
(2,2561)	1:59:A:LEU:HD13	1:56:A:ILE:HA	4	0.19
(2,2557)	1:59:A:LEU:HD13	1:56:A:ILE:HA	4	0.19
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	2	0.19
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	4	0.19
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	5	0.19
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	6	0.19
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	8	0.19
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	2	0.19
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	6	0.19
(2,2511)	1:54:A:VAL:HG22	1:58:A:SER:HB2	8	0.19
(2,2482)	1:50:A:ALA:HB3	1:54:A:VAL:HG11	8	0.19
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	2	0.19
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	2	0.19
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	5	0.19
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG2	2	0.19
(2,2405)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	1	0.19
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	3	0.19
(2,2329)	1:33:A:LYS:HB3	1:33:A:LYS:HE2	6	0.19
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE3	10	0.19
(2,2324)	1:32:A:ILE:HD12	1:31:A:LEU:H	7	0.19
(2,2318)	1:32:A:ILE:HD13	1:9:A:CYS:H	2	0.19
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG23	4	0.19
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG23	5	0.19
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG21	8	0.19
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	1	0.19
(2,2165)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	1	0.19
(2,2147)	1:15:A:ILE:HD12	2:103:B:TYR:HA	4	0.19
(2,2073)	1:7:A:LEU:HD11	1:7:A:LEU:H	1	0.19
(2,2073)	1:7:A:LEU:HD12	1:7:A:LEU:H	5	0.19
(2,2073)	1:7:A:LEU:HD12	1:7:A:LEU:H	7	0.19
(2,2057)	1:4:A:VAL:HG13	2:112:B:LEU:HB3	3	0.19
(2,2057)	1:4:A:VAL:HG12	2:112:B:LEU:HB3	7	0.19
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB3	6	0.19
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	10	0.19
(2,1958)	2:155:B:ILE:HA	2:155:B:ILE:HD13	9	0.19
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	3	0.19
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	5	0.19
(2,1879)	2:143:B:ILE:HG21	2:143:B:ILE:HG12	3	0.19
(2,1866)	2:143:B:ILE:HA	2:143:B:ILE:HG12	7	0.19
(2,1866)	2:143:B:ILE:HA	2:143:B:ILE:HG12	8	0.19
(2,1827)	2:137:B:ASP:HA	2:137:B:ASP:HB3	9	0.19
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB3	9	0.19
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB2	4	0.19
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD3	9	0.19
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	2	0.19
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	6	0.19
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	9	0.19
(2,1639)	2:108:B:LEU:HB3	2:108:B:LEU:HD22	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1601)	1:61:A:CYS:HA	1:61:A:CYS:HB2	1	0.19
(2,1598)	1:57:A:GLY:HA2	1:60:A:ILE:HD11	6	0.19
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG23	10	0.19
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB2	8	0.19
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	2	0.19
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	7	0.19
(2,1536)	1:51:A:LEU:HD13	1:51:A:LEU:HG	8	0.19
(2,1485)	1:39:A:VAL:HG13	1:43:A:TRP:HA	2	0.19
(2,1450)	1:33:A:LYS:HG3	1:33:A:LYS:HD2	4	0.19
(2,1443)	1:33:A:LYS:HA	1:33:A:LYS:HB3	8	0.19
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG3	5	0.19
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG2	7	0.19
(2,1402)	1:26:A:ASP:HB3	1:26:A:ASP:HA	3	0.19
(2,1402)	1:26:A:ASP:HB3	1:26:A:ASP:HA	7	0.19
(2,1381)	1:23:A:VAL:HG11	1:48:A:ALA:HB2	8	0.19
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG22	4	0.19
(2,1337)	1:14:A:LEU:HG	1:56:A:ILE:HG12	6	0.19
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG11	6	0.19
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB3	1	0.19
(2,1230)	2:162:B:LEU:HD11	2:162:B:LEU:HG	2	0.19
(2,1230)	2:162:B:LEU:HD22	2:162:B:LEU:HG	3	0.19
(2,1230)	2:162:B:LEU:HD12	2:162:B:LEU:HG	4	0.19
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	7	0.19
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	7	0.19
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	10	0.19
(2,1179)	2:155:B:ILE:HG23	2:155:B:ILE:HB	3	0.19
(2,1179)	2:155:B:ILE:HG23	2:155:B:ILE:HB	4	0.19
(2,1179)	2:155:B:ILE:HG23	2:155:B:ILE:HB	10	0.19
(2,1133)	2:146:B:LEU:HB3	2:146:B:LEU:HD11	7	0.19
(2,1130)	2:146:B:LEU:HD13	2:146:B:LEU:HG	5	0.19
(2,1130)	2:146:B:LEU:HD12	2:146:B:LEU:HG	7	0.19
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG23	4	0.19
(2,1093)	2:143:B:ILE:HA	2:146:B:LEU:HD13	6	0.19
(2,1063)	2:139:B:LEU:HD21	2:103:B:TYR:HE1	4	0.19
(2,1063)	2:139:B:LEU:HD21	2:103:B:TYR:HE1	10	0.19
(2,1023)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	2	0.19
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	3	0.19
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB3	2	0.19
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG2	9	0.19
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	4	0.19
(2,735)	1:59:A:LEU:HA	1:59:A:LEU:HD21	10	0.19
(2,733)	1:59:A:LEU:HB2	1:56:A:ILE:HA	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG12	5	0.19
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG13	8	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	1	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	2	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	3	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	4	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	5	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	6	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	7	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	8	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	9	0.19
(2,676)	1:49:A:LYS:HB2	1:49:A:LYS:HB3	10	0.19
(2,660)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	2	0.19
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	5	0.19
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	1	0.19
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	2	0.19
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	7	0.19
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	10	0.19
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	5	0.19
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	4	0.19
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	8	0.19
(2,500)	1:26:A:ASP:HA	1:29:A:ASN:HB3	6	0.19
(2,496)	1:25:A:GLU:HB2	1:25:A:GLU:HG3	6	0.19
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG23	9	0.19
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG12	2	0.19
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG12	7	0.19
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG22	7	0.19
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD22	1	0.19
(2,365)	1:7:A:LEU:HA	1:9:A:CYS:HB3	4	0.19
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	10	0.19
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	10	0.19
(2,339)	1:1:A:MET:HB2	1:1:A:MET:HA	6	0.19
(2,333)	2:167:B:ALA:H	2:166:B:PRO:HB3	4	0.19
(2,328)	2:163:B:ALA:H	2:162:B:LEU:HB3	2	0.19
(2,316)	2:154:B:VAL:H	2:154:B:VAL:HG23	10	0.19
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	4	0.19
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB1	9	0.19
(2,247)	2:126:B:ILE:H	2:127:B:LEU:HD12	7	0.19
(2,220)	2:119:B:SER:H	2:119:B:SER:HB3	9	0.19
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	8	0.19
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	10	0.19
(2,199)	2:114:B:GLY:H	2:112:B:LEU:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,151)	1:59:A:LEU:H	1:59:A:LEU:HD22	1	0.19
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD12	10	0.19
(2,109)	1:39:A:VAL:H	1:38:A:ASN:HB3	10	0.19
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	7	0.19
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	5	0.19
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	7	0.19
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	2	0.19
(1,41)	1:45:A:GLY:N	1:41:A:PRO:O	10	0.19
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	6	0.18
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	4	0.18
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	2	0.18
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	4	0.18
(2,4520)	2:145:B:GLU:HG2	2:145:B:GLU:H	6	0.18
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	7	0.18
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	10	0.18
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	2	0.18
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	10	0.18
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	9	0.18
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	5	0.18
(2,4208)	2:165:B:VAL:HA	2:165:B:VAL:HB	9	0.18
(2,4190)	2:132:B:ILE:HA	2:132:B:ILE:HG13	9	0.18
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	5	0.18
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	6	0.18
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	6	0.18
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	4	0.18
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	1	0.18
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	3	0.18
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	6	0.18
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	8	0.18
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	9	0.18
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	6	0.18
(2,3840)	2:122:B:ASP:H	2:122:B:ASP:HB3	10	0.18
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	7	0.18
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	2	0.18
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	5	0.18
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	8	0.18
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	7	0.18
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG23	4	0.18
(2,3466)	2:130:B:VAL:HB	1:27:A:LYS:HD2	6	0.18
(2,3464)	2:129:B:SER:HA	1:34:A:ALA:HA	10	0.18
(2,3432)	2:108:B:LEU:HD22	1:14:A:LEU:HD23	5	0.18
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3429)	2:108:B:LEU:HD22	1:14:A:LEU:HD23	5	0.18
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	7	0.18
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	6	0.18
(2,3388)	1:37:A:VAL:HG23	2:112:B:LEU:HD23	4	0.18
(2,3388)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	6	0.18
(2,3364)	1:31:A:LEU:HD11	2:130:B:VAL:HA	5	0.18
(2,3355)	1:21:A:VAL:HG11	2:132:B:ILE:HB	6	0.18
(2,3322)	1:10:A:ILE:HD11	2:159:B:ILE:HG22	8	0.18
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	7	0.18
(2,3317)	1:8:A:ALA:HB2	2:109:B:LEU:HG	10	0.18
(2,3307)	1:4:A:VAL:HG11	2:112:B:LEU:HA	6	0.18
(2,3287)	2:166:B:PRO:HD3	2:166:B:PRO:HA	7	0.18
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG11	1	0.18
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG11	10	0.18
(2,3252)	2:162:B:LEU:HD11	2:159:B:ILE:HA	9	0.18
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD13	2	0.18
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD12	8	0.18
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD23	1	0.18
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD21	2	0.18
(2,3239)	2:161:B:LYS:HD3	2:161:B:LYS:HA	1	0.18
(2,3238)	2:161:B:LYS:H	2:161:B:LYS:HB2	8	0.18
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	3	0.18
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	4	0.18
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	5	0.18
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	6	0.18
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	8	0.18
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	9	0.18
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	1	0.18
(2,3221)	2:159:B:ILE:HD13	2:158:B:GLY:H	6	0.18
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	8	0.18
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG2	7	0.18
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG2	10	0.18
(2,3078)	2:144:B:SER:H	2:143:B:ILE:HG22	2	0.18
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB3	4	0.18
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	7	0.18
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD12	6	0.18
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD12	7	0.18
(2,2945)	2:132:B:ILE:HD12	2:133:B:GLU:H	2	0.18
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD13	4	0.18
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD13	8	0.18
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	2	0.18
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	7	0.18
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	9	0.18
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	10	0.18
(2,2855)	2:124:B:LYS:HA	2:124:B:LYS:HE2	2	0.18
(2,2851)	2:123:B:ILE:HG21	2:126:B:ILE:H	6	0.18
(2,2842)	2:123:B:ILE:HG23	2:139:B:LEU:H	10	0.18
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB2	5	0.18
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	10	0.18
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	1	0.18
(2,2654)	2:105:B:ALA:HB3	2:162:B:LEU:HD23	10	0.18
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	4	0.18
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	6	0.18
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG13	10	0.18
(2,2589)	1:62:A:ASN:HB3	1:43:A:TRP:HZ2	4	0.18
(2,2588)	1:63:A:VAL:H	1:62:A:ASN:HB3	8	0.18
(2,2561)	1:59:A:LEU:HD13	1:56:A:ILE:HA	9	0.18
(2,2557)	1:59:A:LEU:HD13	1:56:A:ILE:HA	9	0.18
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	1	0.18
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	6	0.18
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	8	0.18
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	10	0.18
(2,2547)	1:59:A:LEU:HB2	1:56:A:ILE:HA	9	0.18
(2,2543)	1:58:A:SER:HB3	1:59:A:LEU:HG	1	0.18
(2,2500)	1:51:A:LEU:HB2	1:51:A:LEU:HD12	5	0.18
(2,2496)	1:51:A:LEU:HB3	1:51:A:LEU:HD22	9	0.18
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD11	2	0.18
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	1	0.18
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	4	0.18
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	9	0.18
(2,2398)	1:8:A:ALA:HB2	1:39:A:VAL:HG21	2	0.18
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	2	0.18
(2,2388)	1:37:A:VAL:HG23	1:38:A:ASN:HB3	10	0.18
(2,2261)	1:25:A:GLU:HG2	1:26:A:ASP:H	3	0.18
(2,2251)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	3	0.18
(2,2245)	1:24:A:THR:HG23	1:27:A:LYS:HE3	5	0.18
(2,2204)	1:20:A:GLU:HG2	1:19:A:ASP:H	1	0.18
(2,2162)	1:16:A:LEU:HD23	1:13:A:ALA:HA	6	0.18
(2,2149)	1:15:A:ILE:HD12	1:15:A:ILE:H	6	0.18
(2,2149)	1:15:A:ILE:HD12	1:15:A:ILE:H	7	0.18
(2,2142)	1:15:A:ILE:HD12	1:15:A:ILE:HA	2	0.18
(2,2142)	1:15:A:ILE:HD13	1:15:A:ILE:HA	5	0.18
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2105)	1:10:A:ILE:HG23	1:10:A:ILE:HG12	2	0.18
(2,2057)	1:4:A:VAL:HG11	2:112:B:LEU:HB3	8	0.18
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG12	5	0.18
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG13	7	0.18
(2,2013)	2:165:B:VAL:HA	2:165:B:VAL:HG22	9	0.18
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB2	10	0.18
(2,1995)	2:162:B:LEU:HA	2:162:B:LEU:HB3	3	0.18
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB1	4	0.18
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	9	0.18
(2,1962)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	10	0.18
(2,1953)	2:155:B:ILE:HA	2:155:B:ILE:HD13	9	0.18
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG2	10	0.18
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	1	0.18
(2,1876)	2:143:B:ILE:HG22	2:147:B:ASN:HB2	3	0.18
(2,1856)	2:142:B:VAL:HA	2:142:B:VAL:HG21	8	0.18
(2,1834)	2:138:B:ARG:HG2	2:138:B:ARG:HD3	3	0.18
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB2	4	0.18
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB2	6	0.18
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB3	10	0.18
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	7	0.18
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	8	0.18
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG23	1	0.18
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG13	3	0.18
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG23	8	0.18
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	4	0.18
(2,1536)	1:51:A:LEU:HD11	1:51:A:LEU:HG	7	0.18
(2,1368)	1:21:A:VAL:HA	1:21:A:VAL:HG23	9	0.18
(2,1242)	2:165:B:VAL:HG13	2:166:B:PRO:HD2	9	0.18
(2,1230)	2:162:B:LEU:HD12	2:162:B:LEU:HG	5	0.18
(2,1230)	2:162:B:LEU:HD11	2:162:B:LEU:HG	7	0.18
(2,1230)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.18
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG21	4	0.18
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG23	7	0.18
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG22	9	0.18
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG23	10	0.18
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	10	0.18
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG22	6	0.18
(2,1075)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.18
(2,1075)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.18
(2,1064)	2:137:B:ASP:HA	2:139:B:LEU:HD13	10	0.18
(2,1063)	2:139:B:LEU:HD21	2:103:B:TYR:HE1	5	0.18
(2,1023)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,951)	2:125:B:LYS:HD2	2:129:B:SER:HB3	6	0.18
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	4	0.18
(2,851)	2:107:B:TYR:HA	2:110:B:ALA:HB2	8	0.18
(2,842)	2:109:B:LEU:HD22	1:12:A:SER:HA	1	0.18
(2,763)	1:43:A:TRP:HD1	1:6:A:GLU:HG3	5	0.18
(2,738)	1:59:A:LEU:HD12	1:59:A:LEU:HG	1	0.18
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	6	0.18
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	10	0.18
(2,719)	1:56:A:ILE:HD11	1:17:A:HIS:HD2	3	0.18
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG13	1	0.18
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG12	6	0.18
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG13	10	0.18
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	1	0.18
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	4	0.18
(2,658)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	9	0.18
(2,658)	1:46:A:LEU:HD21	1:42:A:PHE:HZ	10	0.18
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	9	0.18
(2,615)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	9	0.18
(2,596)	1:37:A:VAL:HG13	2:113:B:GLY:HA2	2	0.18
(2,588)	1:37:A:VAL:HG21	2:112:B:LEU:HG	5	0.18
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	2	0.18
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG3	10	0.18
(2,496)	1:25:A:GLU:HB2	1:25:A:GLU:HG3	10	0.18
(2,493)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	8	0.18
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG21	1	0.18
(2,467)	1:22:A:THR:HA	1:23:A:VAL:HG23	6	0.18
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG22	1	0.18
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG23	2	0.18
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG23	3	0.18
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG23	8	0.18
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG12	1	0.18
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG13	8	0.18
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG22	4	0.18
(2,460)	1:21:A:VAL:HA	1:21:A:VAL:HG23	9	0.18
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE2	9	0.18
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	4	0.18
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD23	10	0.18
(2,347)	1:2:A:ALA:HB1	1:7:A:LEU:HB2	6	0.18
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB3	2	0.18
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB1	3	0.18
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB3	6	0.18
(2,344)	1:2:A:ALA:HB1	1:7:A:LEU:HB2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,340)	1:1:A:MET:HG2	1:1:A:MET:HB2	3	0.18
(2,340)	1:1:A:MET:HG3	1:1:A:MET:HB2	7	0.18
(2,339)	1:1:A:MET:HB3	1:1:A:MET:HA	1	0.18
(2,316)	2:154:B:VAL:H	2:154:B:VAL:HG23	4	0.18
(2,299)	2:146:B:LEU:H	2:146:B:LEU:HD22	6	0.18
(2,279)	2:139:B:LEU:H	2:139:B:LEU:HD13	6	0.18
(2,264)	2:133:B:GLU:H	2:134:B:ALA:HB1	6	0.18
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD13	4	0.18
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD13	8	0.18
(2,244)	2:125:B:LYS:H	2:125:B:LYS:HD3	9	0.18
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	5	0.18
(2,196)	2:113:B:GLY:H	1:37:A:VAL:HG11	1	0.18
(2,169)	1:43:A:TRP:HE1	1:5:A:SER:HB2	3	0.18
(2,36)	1:13:A:ALA:H	1:51:A:LEU:HD13	7	0.18
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	4	0.18
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	8	0.18
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	10	0.18
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	4	0.18
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	6	0.17
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	5	0.17
(2,4556)	2:161:B:LYS:HA	2:161:B:LYS:H	5	0.17
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	1	0.17
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	2	0.17
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	5	0.17
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	10	0.17
(2,4517)	2:144:B:SER:HA	2:143:B:ILE:HB	4	0.17
(2,4512)	2:143:B:ILE:HA	2:146:B:LEU:HG	6	0.17
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	6	0.17
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	7	0.17
(2,4455)	2:124:B:LYS:HA	2:127:B:LEU:HB3	7	0.17
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	1	0.17
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	2	0.17
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	5	0.17
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	7	0.17
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	10	0.17
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	4	0.17
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	8	0.17
(2,4251)	1:15:A:ILE:HA	2:103:B:TYR:HA	2	0.17
(2,4182)	2:124:B:LYS:HA	2:127:B:LEU:HB3	7	0.17
(2,4093)	2:132:B:ILE:HB	2:127:B:LEU:HB2	5	0.17
(2,4083)	2:124:B:LYS:HA	2:127:B:LEU:HB3	7	0.17
(2,4014)	1:14:A:LEU:HG	1:11:A:TYR:HA	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	6	0.17
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	7	0.17
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	9	0.17
(2,3814)	2:116:B:SER:H	2:117:B:SER:H	3	0.17
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	4	0.17
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	7	0.17
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	1	0.17
(2,3528)	1:5:A:SER:H	1:3:A:SER:HA	9	0.17
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	3	0.17
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	4	0.17
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	6	0.17
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	10	0.17
(2,3515)	2:155:B:ILE:HG12	1:7:A:LEU:HD22	10	0.17
(2,3501)	2:159:B:ILE:HD13	1:60:A:ILE:HB	8	0.17
(2,3454)	1:35:A:ALA:HB1	2:126:B:ILE:HD11	4	0.17
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	3	0.17
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	5	0.17
(2,3393)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	7	0.17
(2,3378)	1:35:A:ALA:HB1	2:126:B:ILE:HD11	4	0.17
(2,3377)	1:34:A:ALA:HB2	2:126:B:ILE:HB	8	0.17
(2,3364)	1:31:A:LEU:HD11	2:130:B:VAL:HA	9	0.17
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG13	4	0.17
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG11	4	0.17
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG12	6	0.17
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG11	9	0.17
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	8	0.17
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD12	6	0.17
(2,3250)	2:162:B:LEU:HD23	2:162:B:LEU:HG	8	0.17
(2,3248)	2:162:B:LEU:HB3	2:162:B:LEU:HD21	4	0.17
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	1	0.17
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	2	0.17
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	7	0.17
(2,3222)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.17
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	3	0.17
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	4	0.17
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	5	0.17
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	6	0.17
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	9	0.17
(2,3205)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	5	0.17
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	10	0.17
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB3	2	0.17
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	8	0.17
(2,3013)	2:139:B:LEU:H	2:139:B:LEU:HD13	2	0.17
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	9	0.17
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB1	5	0.17
(2,2976)	2:134:B:ALA:HB3	2:135:B:ASP:HB2	1	0.17
(2,2976)	2:134:B:ALA:HB3	2:135:B:ASP:HB2	2	0.17
(2,2892)	2:126:B:ILE:HG21	2:110:B:ALA:H	10	0.17
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD12	9	0.17
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	1	0.17
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	2	0.17
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	3	0.17
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	9	0.17
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	8	0.17
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	4	0.17
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB2	2	0.17
(2,2709)	2:109:B:LEU:HD22	1:12:A:SER:HA	1	0.17
(2,2706)	1:8:A:ALA:HA	2:109:B:LEU:HD13	2	0.17
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	7	0.17
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	3	0.17
(2,2610)	1:47:A:PHE:HE1	1:43:A:TRP:HZ2	9	0.17
(2,2589)	1:62:A:ASN:HB2	1:43:A:TRP:HZ2	2	0.17
(2,2589)	1:62:A:ASN:HB2	1:43:A:TRP:HZ2	5	0.17
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	8	0.17
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	7	0.17
(2,2551)	1:59:A:LEU:HB2	1:56:A:ILE:HA	9	0.17
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	1	0.17
(2,2496)	1:51:A:LEU:HB3	1:51:A:LEU:HD22	3	0.17
(2,2496)	1:51:A:LEU:HB3	1:51:A:LEU:HD21	4	0.17
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD13	3	0.17
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD11	7	0.17
(2,2478)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	6	0.17
(2,2477)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	9	0.17
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG2	1	0.17
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	1	0.17
(2,2346)	1:34:A:ALA:HB1	2:126:B:ILE:HD12	3	0.17
(2,2328)	1:33:A:LYS:HB2	1:33:A:LYS:HD2	2	0.17
(2,2318)	1:32:A:ILE:HD13	1:9:A:CYS:H	10	0.17
(2,2285)	1:28:A:ILE:HA	1:31:A:LEU:HD22	4	0.17
(2,2244)	1:24:A:THR:HG22	1:24:A:THR:HA	2	0.17
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG21	10	0.17
(2,2238)	1:23:A:VAL:HG13	1:51:A:LEU:H	6	0.17
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG23	5	0.17
(2,2165)	1:16:A:LEU:HD21	1:27:A:LYS:HB3	4	0.17
(2,2149)	1:15:A:ILE:HD12	1:15:A:ILE:H	8	0.17
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE1	10	0.17
(2,2057)	1:4:A:VAL:HG12	2:112:B:LEU:HB3	4	0.17
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG22	1	0.17
(2,1996)	2:162:B:LEU:HA	2:104:B:VAL:HG12	7	0.17
(2,1988)	2:161:B:LYS:HD3	2:161:B:LYS:HA	7	0.17
(2,1988)	2:161:B:LYS:HD3	2:161:B:LYS:HA	10	0.17
(2,1967)	2:157:B:GLN:HA	2:157:B:GLN:HG2	6	0.17
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	2	0.17
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	7	0.17
(2,1962)	2:155:B:ILE:HG21	2:155:B:ILE:HG13	4	0.17
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	2	0.17
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	7	0.17
(2,1757)	2:125:B:LYS:HD3	2:125:B:LYS:HG2	4	0.17
(2,1742)	2:134:B:ALA:HB3	2:124:B:LYS:HA	9	0.17
(2,1742)	2:134:B:ALA:HB1	2:124:B:LYS:HA	10	0.17
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	3	0.17
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	1	0.17
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	5	0.17
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	10	0.17
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG21	7	0.17
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	10	0.17
(2,1536)	1:51:A:LEU:HD12	1:51:A:LEU:HG	10	0.17
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	4	0.17
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	8	0.17
(2,1485)	1:39:A:VAL:HG13	1:43:A:TRP:HA	5	0.17
(2,1402)	1:26:A:ASP:HB2	1:26:A:ASP:HA	5	0.17
(2,1402)	1:26:A:ASP:HB3	1:26:A:ASP:HA	10	0.17
(2,1375)	1:22:A:THR:HB	1:22:A:THR:HG22	9	0.17
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	3	0.17
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	7	0.17
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG13	4	0.17
(2,1230)	2:162:B:LEU:HD11	2:162:B:LEU:HG	1	0.17
(2,1230)	2:162:B:LEU:HD11	2:162:B:LEU:HG	9	0.17
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	4	0.17
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	10	0.17
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG22	2	0.17
(2,1217)	2:159:B:ILE:HA	2:159:B:ILE:HG23	8	0.17
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	3	0.17
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	1	0.17
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG12	8	0.17
(2,1179)	2:155:B:ILE:HG21	2:155:B:ILE:HB	8	0.17
(2,1175)	2:154:B:VAL:HG22	2:154:B:VAL:HA	7	0.17
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	4	0.17
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	6	0.17
(2,1149)	2:151:B:ILE:HB	2:151:B:ILE:HD13	7	0.17
(2,1142)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	6	0.17
(2,1108)	2:143:B:ILE:HB	2:143:B:ILE:HG22	7	0.17
(2,1084)	2:103:B:TYR:HB2	2:142:B:VAL:HG11	1	0.17
(2,1076)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.17
(2,1076)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.17
(2,1075)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.17
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB3	10	0.17
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	1	0.17
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	8	0.17
(2,851)	2:107:B:TYR:HA	2:110:B:ALA:HB2	2	0.17
(2,851)	2:107:B:TYR:HA	2:110:B:ALA:HB2	6	0.17
(2,842)	2:109:B:LEU:HD23	1:12:A:SER:HA	8	0.17
(2,792)	2:104:B:VAL:HG23	2:146:B:LEU:HD22	2	0.17
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	5	0.17
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	1	0.17
(2,773)	2:101:B:MET:HE3	2:101:B:MET:HG2	1	0.17
(2,763)	1:43:A:TRP:HD1	1:6:A:GLU:HG3	9	0.17
(2,752)	1:61:A:CYS:HB2	1:60:A:ILE:HG21	8	0.17
(2,719)	1:56:A:ILE:HD11	1:17:A:HIS:HD2	5	0.17
(2,719)	1:56:A:ILE:HD13	1:17:A:HIS:HD2	7	0.17
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	2	0.17
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	10	0.17
(2,673)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	7	0.17
(2,658)	1:46:A:LEU:HD22	1:42:A:PHE:HZ	3	0.17
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	2	0.17
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	3	0.17
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	3	0.17
(2,625)	1:41:A:PRO:HA	1:41:A:PRO:HD3	5	0.17
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	6	0.17
(2,620)	1:40:A:GLU:HG3	1:43:A:TRP:HD1	6	0.17
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	10	0.17
(2,567)	1:34:A:ALA:HB1	2:126:B:ILE:HD12	3	0.17
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG2	3	0.17
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG3	4	0.17
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG2	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB3	3	0.17
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB3	3	0.17
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG2	1	0.17
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG3	5	0.17
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG2	7	0.17
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG21	6	0.17
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG22	7	0.17
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG23	10	0.17
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG12	4	0.17
(2,464)	1:21:A:VAL:HB	1:21:A:VAL:HG13	9	0.17
(2,383)	1:10:A:ILE:HA	1:13:A:ALA:HB2	6	0.17
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	4	0.17
(2,357)	1:4:A:VAL:HG11	2:112:B:LEU:HA	10	0.17
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB2	1	0.17
(2,329)	2:164:B:SER:H	2:162:B:LEU:HB3	5	0.17
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	8	0.17
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	5	0.17
(2,266)	2:134:B:ALA:H	2:133:B:GLU:HG2	1	0.17
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD12	9	0.17
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	9	0.17
(2,220)	2:119:B:SER:H	2:119:B:SER:HB3	10	0.17
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	1	0.17
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	2	0.17
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	7	0.17
(2,130)	1:48:A:ALA:H	1:49:A:LYS:HB2	2	0.17
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	2	0.17
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	3	0.17
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	10	0.17
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	2	0.17
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	6	0.17
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	2	0.17
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	3	0.17
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	5	0.17
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	6	0.17
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	7	0.17
(1,81)	2:129:B:SER:N	2:125:B:LYS:O	1	0.17
(1,75)	2:126:B:ILE:N	2:122:B:ASP:O	4	0.17
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	1	0.16
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	9	0.16
(2,4524)	2:146:B:LEU:H	2:146:B:LEU:HG	3	0.16
(2,4520)	2:145:B:GLU:HG2	2:145:B:GLU:H	5	0.16
(2,4517)	2:144:B:SER:HA	2:143:B:ILE:HB	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	8	0.16
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	1	0.16
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	2	0.16
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	3	0.16
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	4	0.16
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	5	0.16
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	8	0.16
(2,4490)	2:137:B:ASP:H	2:137:B:ASP:HA	9	0.16
(2,4446)	2:120:B:ALA:HA	2:140:B:ASN:HA	1	0.16
(2,4422)	2:108:B:LEU:HA	2:107:B:TYR:H	5	0.16
(2,4342)	1:41:A:PRO:HA	1:40:A:GLU:H	7	0.16
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	2	0.16
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	3	0.16
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	6	0.16
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	8	0.16
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	9	0.16
(2,4084)	2:124:B:LYS:HA	2:124:B:LYS:HD2	6	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	1	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	2	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	3	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	4	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	5	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	6	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	7	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	8	0.16
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	10	0.16
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	10	0.16
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	4	0.16
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	10	0.16
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	2	0.16
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	5	0.16
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	10	0.16
(2,3804)	2:115:B:ASN:H	2:116:B:SER:HA	8	0.16
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	7	0.16
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	4	0.16
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	9	0.16
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	2	0.16
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	5	0.16
(2,3504)	1:59:A:LEU:HD11	2:159:B:ILE:HG21	1	0.16
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	2	0.16
(2,3413)	2:101:B:MET:HE2	1:14:A:LEU:HB2	3	0.16
(2,3387)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3364)	1:31:A:LEU:HD12	2:130:B:VAL:HA	7	0.16
(2,3317)	1:8:A:ALA:HB2	2:109:B:LEU:HG	3	0.16
(2,3317)	1:8:A:ALA:HB1	2:109:B:LEU:HG	9	0.16
(2,3308)	1:4:A:VAL:HG11	2:112:B:LEU:HD21	10	0.16
(2,3303)	1:4:A:VAL:HG22	2:112:B:LEU:HD11	9	0.16
(2,3302)	1:4:A:VAL:HB	2:112:B:LEU:HD23	4	0.16
(2,3269)	2:165:B:VAL:H	2:165:B:VAL:HG22	9	0.16
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG12	2	0.16
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG13	3	0.16
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG11	8	0.16
(2,3250)	2:162:B:LEU:HD12	2:162:B:LEU:HG	6	0.16
(2,3248)	2:162:B:LEU:HB3	2:162:B:LEU:HD21	10	0.16
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	7	0.16
(2,3238)	2:161:B:LYS:H	2:161:B:LYS:HB2	2	0.16
(2,3234)	2:159:B:ILE:HG23	1:61:A:CYS:H	9	0.16
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	1	0.16
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	2	0.16
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	7	0.16
(2,3220)	2:159:B:ILE:HD11	2:159:B:ILE:HG13	10	0.16
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG3	8	0.16
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB1	4	0.16
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	9	0.16
(2,3111)	2:104:B:VAL:HA	2:146:B:LEU:HD22	1	0.16
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB3	5	0.16
(2,3079)	2:143:B:ILE:HA	2:143:B:ILE:HG21	4	0.16
(2,3079)	2:143:B:ILE:HA	2:143:B:ILE:HG21	10	0.16
(2,3072)	2:143:B:ILE:HG23	2:119:B:SER:HB3	8	0.16
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD13	2	0.16
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD11	8	0.16
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD12	9	0.16
(2,3011)	2:137:B:ASP:HB3	2:138:B:ARG:HG2	4	0.16
(2,3011)	2:137:B:ASP:HB3	2:138:B:ARG:HG2	5	0.16
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	2	0.16
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB1	1	0.16
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	7	0.16
(2,2976)	2:134:B:ALA:HB2	2:135:B:ASP:HB3	6	0.16
(2,2861)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	10	0.16
(2,2851)	2:123:B:ILE:HG22	2:126:B:ILE:H	7	0.16
(2,2842)	2:123:B:ILE:HG22	2:139:B:LEU:H	9	0.16
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	7	0.16
(2,2818)	2:120:B:ALA:HB1	2:141:B:LYS:H	4	0.16
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	7	0.16
(2,2742)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	7	0.16
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB3	1	0.16
(2,2727)	2:115:B:ASN:H	2:111:B:ALA:HB3	4	0.16
(2,2709)	2:109:B:LEU:HD23	1:12:A:SER:HA	8	0.16
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	2	0.16
(2,2641)	2:104:B:VAL:HA	2:104:B:VAL:HG13	5	0.16
(2,2626)	2:101:B:MET:HE2	2:102:B:ARG:H	2	0.16
(2,2594)	1:63:A:VAL:HB	1:63:A:VAL:HG22	5	0.16
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	7	0.16
(2,2540)	1:54:A:VAL:HG23	1:58:A:SER:HB2	5	0.16
(2,2503)	1:53:A:ASN:H	1:53:A:ASN:HB3	2	0.16
(2,2493)	1:51:A:LEU:H	1:51:A:LEU:HD13	5	0.16
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	8	0.16
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	8	0.16
(2,2458)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	7	0.16
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG2	7	0.16
(2,2413)	1:40:A:GLU:HG2	1:43:A:TRP:HD1	3	0.16
(2,2396)	1:39:A:VAL:H	1:39:A:VAL:HG22	7	0.16
(2,2379)	1:8:A:ALA:HB3	1:37:A:VAL:HG22	2	0.16
(2,2368)	1:37:A:VAL:HG13	2:113:B:GLY:HA2	10	0.16
(2,2346)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	5	0.16
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE3	5	0.16
(2,2255)	1:25:A:GLU:HG2	1:26:A:ASP:HA	1	0.16
(2,2251)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	4	0.16
(2,2244)	1:24:A:THR:HG22	1:24:A:THR:HA	6	0.16
(2,2244)	1:24:A:THR:HG22	1:24:A:THR:HA	8	0.16
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG23	2	0.16
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG13	3	0.16
(2,2204)	1:20:A:GLU:HG2	1:19:A:ASP:H	9	0.16
(2,2159)	1:16:A:LEU:H	1:16:A:LEU:HD12	4	0.16
(2,2073)	1:7:A:LEU:HD12	1:7:A:LEU:H	9	0.16
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG21	2	0.16
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG23	7	0.16
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG13	1	0.16
(2,1995)	2:162:B:LEU:HA	2:162:B:LEU:HB3	5	0.16
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	1	0.16
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	3	0.16
(2,1945)	2:149:B:LYS:HB3	2:154:B:VAL:HG21	7	0.16
(2,1944)	2:154:B:VAL:HG12	2:154:B:VAL:HA	2	0.16
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	8	0.16
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	3	0.16
(2,1792)	2:130:B:VAL:HG22	2:127:B:LEU:HA	6	0.16
(2,1718)	2:121:B:LYS:HB3	2:121:B:LYS:HG2	3	0.16
(2,1678)	2:110:B:ALA:HB1	2:118:B:PRO:HA	6	0.16
(2,1665)	1:4:A:VAL:HB	2:112:B:LEU:HD23	4	0.16
(2,1624)	2:104:B:VAL:HA	2:104:B:VAL:HG13	5	0.16
(2,1613)	2:101:B:MET:HE2	2:101:B:MET:HG2	2	0.16
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG13	2	0.16
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG13	6	0.16
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG13	7	0.16
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG11	8	0.16
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG22	2	0.16
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG21	6	0.16
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB2	9	0.16
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	6	0.16
(2,1567)	1:56:A:ILE:HD12	1:59:A:LEU:HG	3	0.16
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	1	0.16
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	3	0.16
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	10	0.16
(2,1450)	1:33:A:LYS:HG2	1:33:A:LYS:HD3	1	0.16
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG3	4	0.16
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG2	6	0.16
(2,1387)	1:23:A:VAL:HG11	1:48:A:ALA:HB1	7	0.16
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB2	9	0.16
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	2	0.16
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD13	1	0.16
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD13	7	0.16
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD11	10	0.16
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	1	0.16
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	2	0.16
(2,1191)	2:157:B:GLN:HB2	2:154:B:VAL:HA	6	0.16
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	5	0.16
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	8	0.16
(2,1179)	2:155:B:ILE:HG23	2:155:B:ILE:HB	1	0.16
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	9	0.16
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	1	0.16
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	7	0.16
(2,1130)	2:146:B:LEU:HD22	2:146:B:LEU:HG	4	0.16
(2,1115)	2:144:B:SER:HA	2:147:B:ASN:HB2	4	0.16
(2,1076)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.16
(2,1059)	2:139:B:LEU:HD12	2:120:B:ALA:HA	4	0.16
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1038)	2:136:B:ASP:HA	2:136:B:ASP:HB2	5	0.16
(2,1034)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	3	0.16
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	4	0.16
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	6	0.16
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	8	0.16
(2,956)	2:125:B:LYS:HA	2:125:B:LYS:HG2	9	0.16
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG2	8	0.16
(2,920)	2:122:B:ASP:HA	2:125:B:LYS:HG2	2	0.16
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	5	0.16
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	9	0.16
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	3	0.16
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	7	0.16
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	9	0.16
(2,790)	2:104:B:VAL:HG13	2:146:B:LEU:HD22	5	0.16
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	4	0.16
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG11	2	0.16
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG11	3	0.16
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG11	7	0.16
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG23	1	0.16
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG13	3	0.16
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	2	0.16
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	5	0.16
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	10	0.16
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	1	0.16
(2,726)	1:58:A:SER:HB2	1:58:A:SER:HA	9	0.16
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG12	3	0.16
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	3	0.16
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	5	0.16
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	8	0.16
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	7	0.16
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	9	0.16
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	4	0.16
(2,620)	1:40:A:GLU:HG3	1:43:A:TRP:HD1	4	0.16
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	8	0.16
(2,588)	1:37:A:VAL:HG22	2:112:B:LEU:HG	2	0.16
(2,567)	1:34:A:ALA:HB2	2:126:B:ILE:HG23	5	0.16
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB3	1	0.16
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB3	1	0.16
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB3	6	0.16
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG22	4	0.16
(2,426)	1:15:A:ILE:HG21	1:18:A:ASP:HB3	8	0.16
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD23	10	0.16
(2,351)	1:4:A:VAL:HA	1:7:A:LEU:HD21	6	0.16
(2,330)	2:164:B:SER:H	2:164:B:SER:HB3	9	0.16
(2,312)	2:153:B:ASP:H	2:152:B:GLU:HG3	3	0.16
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	9	0.16
(2,282)	2:140:B:ASN:H	2:141:B:LYS:HB3	10	0.16
(2,229)	2:121:B:LYS:H	2:121:B:LYS:HE3	2	0.16
(2,220)	2:119:B:SER:H	2:119:B:SER:HB3	1	0.16
(2,216)	2:117:B:SER:H	2:117:B:SER:HB3	9	0.16
(2,208)	2:115:B:ASN:H	2:111:B:ALA:HB3	4	0.16
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG11	2	0.16
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG12	9	0.16
(2,142)	1:53:A:ASN:H	1:53:A:ASN:HB3	2	0.16
(2,141)	1:53:A:ASN:H	1:53:A:ASN:HB3	2	0.16
(2,128)	1:48:A:ALA:H	1:28:A:ILE:HD12	8	0.16
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	5	0.16
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	8	0.16
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	9	0.16
(2,109)	1:39:A:VAL:H	1:38:A:ASN:HB3	3	0.16
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD23	7	0.16
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	8	0.16
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	1	0.16
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	4	0.16
(1,84)	2:139:B:LEU:H	2:135:B:ASP:O	8	0.16
(1,81)	2:129:B:SER:N	2:125:B:LYS:O	10	0.16
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	1	0.16
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	6	0.16
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	8	0.16
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	1	0.16
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	3	0.16
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	2	0.16
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	5	0.16
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	6	0.16
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	7	0.16
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	8	0.16
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	9	0.16
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	1	0.16
(1,13)	1:13:A:ALA:N	1:9:A:CYS:O	6	0.16
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	7	0.15
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	10	0.15
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	6	0.15
(2,4524)	2:146:B:LEU:H	2:146:B:LEU:HG	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4517)	2:144:B:SER:HA	2:143:B:ILE:HB	1	0.15
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	6	0.15
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	1	0.15
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	9	0.15
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	2	0.15
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	6	0.15
(2,4251)	1:15:A:ILE:HA	2:103:B:TYR:HA	1	0.15
(2,4251)	1:15:A:ILE:HA	2:103:B:TYR:HA	10	0.15
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	1	0.15
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	2	0.15
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	5	0.15
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	10	0.15
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	2	0.15
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	5	0.15
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	7	0.15
(2,4204)	2:155:B:ILE:HD12	2:155:B:ILE:HB	9	0.15
(2,4191)	2:138:B:ARG:HA	2:138:B:ARG:HG2	6	0.15
(2,4136)	1:22:A:THR:HA	1:22:A:THR:HB	6	0.15
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	4	0.15
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	2	0.15
(2,4035)	1:39:A:VAL:HA	1:39:A:VAL:HB	9	0.15
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	2	0.15
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	3	0.15
(2,3954)	2:143:B:ILE:H	2:107:B:TYR:HE2	6	0.15
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	2	0.15
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	5	0.15
(2,3842)	2:122:B:ASP:H	2:119:B:SER:HA	6	0.15
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	6	0.15
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	7	0.15
(2,3762)	1:43:A:TRP:HE1	1:40:A:GLU:H	10	0.15
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	3	0.15
(2,3526)	1:5:A:SER:H	1:6:A:GLU:HA	9	0.15
(2,3508)	1:10:A:ILE:HG23	2:159:B:ILE:HG23	4	0.15
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	3	0.15
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	7	0.15
(2,3388)	1:37:A:VAL:HG23	2:112:B:LEU:HD22	7	0.15
(2,3387)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	6	0.15
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	10	0.15
(2,3317)	1:8:A:ALA:HB1	2:109:B:LEU:HG	2	0.15
(2,3308)	1:4:A:VAL:HG22	2:112:B:LEU:HD11	2	0.15
(2,3302)	1:4:A:VAL:HB	2:112:B:LEU:HD21	10	0.15
(2,3301)	1:2:A:ALA:HB3	2:152:B:GLU:HA	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG12	5	0.15
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG13	5	0.15
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	3	0.15
(2,3256)	2:162:B:LEU:HD13	2:159:B:ILE:HA	3	0.15
(2,3256)	2:162:B:LEU:HD13	2:159:B:ILE:HA	4	0.15
(2,3250)	2:162:B:LEU:HD11	2:162:B:LEU:HG	2	0.15
(2,3250)	2:162:B:LEU:HD22	2:162:B:LEU:HG	3	0.15
(2,3250)	2:162:B:LEU:HD12	2:162:B:LEU:HG	4	0.15
(2,3248)	2:162:B:LEU:HB3	2:162:B:LEU:HD21	7	0.15
(2,3238)	2:161:B:LYS:H	2:161:B:LYS:HB2	1	0.15
(2,3234)	2:159:B:ILE:HG22	1:61:A:CYS:H	4	0.15
(2,3234)	2:159:B:ILE:HG21	1:61:A:CYS:H	6	0.15
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	1	0.15
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	2	0.15
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	7	0.15
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB2	1	0.15
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB2	4	0.15
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB3	6	0.15
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB3	7	0.15
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB2	8	0.15
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB2	9	0.15
(2,3079)	2:143:B:ILE:HA	2:143:B:ILE:HG21	1	0.15
(2,3074)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	3	0.15
(2,3074)	2:143:B:ILE:HG23	2:143:B:ILE:HD13	10	0.15
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	9	0.15
(2,3044)	2:142:B:VAL:HA	2:142:B:VAL:HG21	1	0.15
(2,3044)	2:142:B:VAL:HA	2:142:B:VAL:HG21	10	0.15
(2,3013)	2:139:B:LEU:H	2:139:B:LEU:HD13	6	0.15
(2,3011)	2:137:B:ASP:HB3	2:138:B:ARG:HG2	7	0.15
(2,2980)	2:134:B:ALA:HB3	2:135:B:ASP:H	4	0.15
(2,2972)	2:134:B:ALA:HB3	2:139:B:LEU:HD22	7	0.15
(2,2872)	2:125:B:LYS:HD2	2:125:B:LYS:HB3	9	0.15
(2,2860)	2:124:B:LYS:HG3	2:124:B:LYS:HE2	6	0.15
(2,2820)	2:120:B:ALA:HB3	2:140:B:ASN:HB2	4	0.15
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	6	0.15
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB3	10	0.15
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	1	0.15
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	2	0.15
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	6	0.15
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB3	3	0.15
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB1	7	0.15
(2,2590)	1:62:A:ASN:H	1:62:A:ASN:HB3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	8	0.15
(2,2496)	1:51:A:LEU:HB2	1:51:A:LEU:HD11	7	0.15
(2,2482)	1:50:A:ALA:HB2	1:54:A:VAL:HG22	1	0.15
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	3	0.15
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	10	0.15
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	1	0.15
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	4	0.15
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	10	0.15
(2,2458)	1:46:A:LEU:HD21	1:42:A:PHE:HD1	2	0.15
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	8	0.15
(2,2388)	1:37:A:VAL:HG21	1:38:A:ASN:HB3	7	0.15
(2,2374)	1:37:A:VAL:HA	1:37:A:VAL:HG23	6	0.15
(2,2324)	1:32:A:ILE:HD12	1:31:A:LEU:H	6	0.15
(2,2267)	1:26:A:ASP:HB3	1:30:A:ALA:HB2	5	0.15
(2,2258)	1:25:A:GLU:HG3	1:48:A:ALA:HB3	7	0.15
(2,2245)	1:24:A:THR:HG23	1:27:A:LYS:HE3	9	0.15
(2,2244)	1:24:A:THR:HG22	1:24:A:THR:HA	3	0.15
(2,2222)	1:22:A:THR:HA	1:22:A:THR:HG21	9	0.15
(2,2218)	1:22:A:THR:HA	1:22:A:THR:HG21	6	0.15
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG21	10	0.15
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG13	5	0.15
(2,2204)	1:20:A:GLU:HG2	1:19:A:ASP:H	4	0.15
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE2	7	0.15
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG21	9	0.15
(2,2045)	1:4:A:VAL:HA	1:7:A:LEU:HD21	9	0.15
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG13	8	0.15
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB3	7	0.15
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB3	9	0.15
(2,1967)	2:157:B:GLN:HA	2:157:B:GLN:HG2	4	0.15
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB2	5	0.15
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB1	6	0.15
(2,1944)	2:154:B:VAL:HG12	2:154:B:VAL:HA	10	0.15
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	10	0.15
(2,1857)	2:142:B:VAL:HA	2:142:B:VAL:HG21	8	0.15
(2,1757)	2:125:B:LYS:HD2	2:125:B:LYS:HG3	3	0.15
(2,1731)	2:123:B:ILE:HD13	2:118:B:PRO:HD2	5	0.15
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB3	3	0.15
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB2	5	0.15
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	8	0.15
(2,1678)	2:110:B:ALA:HB1	2:118:B:PRO:HA	5	0.15
(2,1665)	1:4:A:VAL:HB	2:112:B:LEU:HD21	10	0.15
(2,1641)	2:108:B:LEU:HD21	2:155:B:ILE:HG21	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1613)	2:101:B:MET:HE2	2:101:B:MET:HG2	6	0.15
(2,1605)	1:63:A:VAL:HA	1:63:A:VAL:HG11	5	0.15
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG21	1	0.15
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG22	5	0.15
(2,1574)	1:59:A:LEU:HA	1:62:A:ASN:HB2	7	0.15
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	1	0.15
(2,1568)	1:58:A:SER:HB2	1:58:A:SER:HA	9	0.15
(2,1567)	1:56:A:ILE:HD13	1:59:A:LEU:HG	2	0.15
(2,1567)	1:56:A:ILE:HD11	1:59:A:LEU:HG	7	0.15
(2,1545)	1:53:A:ASN:HA	1:53:A:ASN:HB3	5	0.15
(2,1540)	1:47:A:PHE:HA	1:51:A:LEU:HD13	4	0.15
(2,1536)	1:51:A:LEU:HD12	1:51:A:LEU:HG	9	0.15
(2,1530)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	6	0.15
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	5	0.15
(2,1523)	1:49:A:LYS:HA	1:49:A:LYS:HB3	9	0.15
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG2	3	0.15
(2,1418)	1:29:A:ASN:HA	1:29:A:ASN:HB3	2	0.15
(2,1418)	1:29:A:ASN:HA	1:29:A:ASN:HB3	5	0.15
(2,1392)	1:24:A:THR:HG22	1:24:A:THR:HA	2	0.15
(2,1373)	1:22:A:THR:HG23	1:21:A:VAL:HB	9	0.15
(2,1370)	1:19:A:ASP:HB3	1:21:A:VAL:HG13	9	0.15
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	5	0.15
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB3	2	0.15
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB3	6	0.15
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	6	0.15
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	10	0.15
(2,1236)	2:164:B:SER:HA	2:164:B:SER:HB2	2	0.15
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD12	4	0.15
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	6	0.15
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	2	0.15
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	3	0.15
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	4	0.15
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	6	0.15
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	1	0.15
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	5	0.15
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	6	0.15
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	7	0.15
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	10	0.15
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	2	0.15
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	5	0.15
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	8	0.15
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1107)	2:143:B:ILE:HG21	2:143:B:ILE:HG12	3	0.15
(2,1105)	2:143:B:ILE:HG21	2:143:B:ILE:HD11	3	0.15
(2,1105)	2:143:B:ILE:HG23	2:143:B:ILE:HD13	10	0.15
(2,1093)	2:143:B:ILE:HA	2:146:B:LEU:HD13	1	0.15
(2,1090)	2:142:B:VAL:HG22	2:146:B:LEU:HD22	5	0.15
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG12	4	0.15
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	2	0.15
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	5	0.15
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	10	0.15
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	4	0.15
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB3	3	0.15
(2,800)	2:105:B:ALA:HB2	2:101:B:MET:HG2	6	0.15
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	10	0.15
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	5	0.15
(2,761)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	6	0.15
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG11	1	0.15
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG12	8	0.15
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG12	9	0.15
(2,735)	1:59:A:LEU:HA	1:59:A:LEU:HD21	2	0.15
(2,735)	1:59:A:LEU:HA	1:59:A:LEU:HD21	4	0.15
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG12	2	0.15
(2,704)	1:54:A:VAL:HG21	1:58:A:SER:HB3	4	0.15
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	10	0.15
(2,670)	1:49:A:LYS:HA	1:49:A:LYS:HB2	6	0.15
(2,670)	1:49:A:LYS:HA	1:49:A:LYS:HB2	7	0.15
(2,660)	1:46:A:LEU:HD22	1:42:A:PHE:HD1	8	0.15
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD11	5	0.15
(2,628)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	6	0.15
(2,596)	1:37:A:VAL:HG13	2:113:B:GLY:HA2	10	0.15
(2,589)	1:37:A:VAL:HA	1:37:A:VAL:HG23	6	0.15
(2,588)	1:37:A:VAL:HG23	2:112:B:LEU:HG	8	0.15
(2,588)	1:37:A:VAL:HG21	2:112:B:LEU:HG	9	0.15
(2,588)	1:37:A:VAL:HG22	2:112:B:LEU:HG	10	0.15
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	5	0.15
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG3	2	0.15
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB3	6	0.15
(2,502)	1:26:A:ASP:HB3	1:30:A:ALA:HB2	5	0.15
(2,466)	1:21:A:VAL:HA	1:21:A:VAL:HG23	9	0.15
(2,426)	1:15:A:ILE:HG21	1:18:A:ASP:HB3	7	0.15
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE2	3	0.15
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB2	5	0.15
(2,334)	2:167:B:ALA:H	2:167:B:ALA:HB3	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,316)	2:154:B:VAL:H	2:154:B:VAL:HG23	2	0.15
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	4	0.15
(2,308)	2:150:B:ASN:H	2:154:B:VAL:H	10	0.15
(2,304)	2:149:B:LYS:H	2:149:B:LYS:HE2	3	0.15
(2,299)	2:146:B:LEU:H	2:146:B:LEU:HD22	10	0.15
(2,220)	2:119:B:SER:H	2:119:B:SER:HB3	7	0.15
(2,214)	2:117:B:SER:H	2:117:B:SER:HB3	3	0.15
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	2	0.15
(2,196)	2:113:B:GLY:H	1:37:A:VAL:HG13	3	0.15
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG12	5	0.15
(2,157)	1:62:A:ASN:H	1:62:A:ASN:HB3	3	0.15
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	7	0.15
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	4	0.15
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	7	0.15
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	10	0.15
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	1	0.15
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	5	0.15
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	1	0.15
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	2	0.15
(1,81)	2:129:B:SER:N	2:125:B:LYS:O	2	0.15
(1,68)	2:113:B:GLY:H	2:109:B:LEU:O	1	0.15
(1,68)	2:113:B:GLY:H	2:109:B:LEU:O	3	0.15
(1,67)	2:113:B:GLY:N	2:109:B:LEU:O	1	0.15
(1,67)	2:113:B:GLY:N	2:109:B:LEU:O	3	0.15
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	3	0.15
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	3	0.15
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	6	0.15
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	7	0.15
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	7	0.15
(1,25)	1:28:A:ILE:N	1:24:A:THR:O	2	0.15
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	3	0.15
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	10	0.15
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	6	0.15
(2,4557)	2:161:B:LYS:HD2	2:161:B:LYS:H	9	0.14
(2,4512)	2:143:B:ILE:HA	2:146:B:LEU:HG	2	0.14
(2,4512)	2:143:B:ILE:HA	2:146:B:LEU:HG	5	0.14
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	3	0.14
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	9	0.14
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	8	0.14
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	1	0.14
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	3	0.14
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	10	0.14
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	6	0.14
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	7	0.14
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	8	0.14
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	1	0.14
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	7	0.14
(2,4136)	1:22:A:THR:HA	1:22:A:THR:HB	4	0.14
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	5	0.14
(2,4006)	2:169:B:GLY:H	2:168:B:GLY:H	7	0.14
(2,4001)	2:164:B:SER:H	2:163:B:ALA:HA	2	0.14
(2,3852)	2:124:B:LYS:H	2:125:B:LYS:HA	5	0.14
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	1	0.14
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	4	0.14
(2,3728)	1:55:A:ASN:H	1:54:A:VAL:H	9	0.14
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	1	0.14
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	5	0.14
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	6	0.14
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	10	0.14
(2,3504)	1:59:A:LEU:HD12	2:159:B:ILE:HG21	9	0.14
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	8	0.14
(2,3401)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	10	0.14
(2,3393)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	1	0.14
(2,3393)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	3	0.14
(2,3371)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	4	0.14
(2,3364)	1:31:A:LEU:HD13	2:130:B:VAL:HA	4	0.14
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	1	0.14
(2,3303)	1:4:A:VAL:HG22	2:112:B:LEU:HD11	8	0.14
(2,3297)	1:1:A:MET:HE1	2:152:B:GLU:HA	8	0.14
(2,3270)	2:165:B:VAL:HG12	2:161:B:LYS:HG2	3	0.14
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	5	0.14
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD13	3	0.14
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD11	9	0.14
(2,3250)	2:162:B:LEU:HD12	2:162:B:LEU:HG	5	0.14
(2,3250)	2:162:B:LEU:HD11	2:162:B:LEU:HG	7	0.14
(2,3250)	2:162:B:LEU:HD11	2:162:B:LEU:HG	10	0.14
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD13	9	0.14
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	4	0.14
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	10	0.14
(2,3239)	2:161:B:LYS:HD3	2:161:B:LYS:HA	7	0.14
(2,3239)	2:161:B:LYS:HD3	2:161:B:LYS:HA	10	0.14
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG3	5	0.14
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB2	5	0.14
(2,3168)	2:154:B:VAL:HG22	2:154:B:VAL:HA	7	0.14
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	6	0.14
(2,3108)	2:146:B:LEU:HD22	2:145:B:GLU:HB2	3	0.14
(2,3085)	2:144:B:SER:H	2:144:B:SER:HB2	7	0.14
(2,3074)	2:143:B:ILE:HG23	2:143:B:ILE:HD13	1	0.14
(2,3070)	2:120:B:ALA:H	2:143:B:ILE:HG23	2	0.14
(2,3069)	2:143:B:ILE:H	2:143:B:ILE:HD11	5	0.14
(2,3044)	2:142:B:VAL:HA	2:142:B:VAL:HG21	4	0.14
(2,2992)	2:137:B:ASP:HA	2:140:B:ASN:HB3	1	0.14
(2,2873)	2:125:B:LYS:HA	2:125:B:LYS:HG3	1	0.14
(2,2872)	2:125:B:LYS:HD2	2:125:B:LYS:HB3	6	0.14
(2,2872)	2:125:B:LYS:HD2	2:125:B:LYS:HB3	8	0.14
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	1	0.14
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	8	0.14
(2,2861)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	1	0.14
(2,2779)	2:117:B:SER:H	2:117:B:SER:HB3	9	0.14
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	10	0.14
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB2	3	0.14
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	1	0.14
(2,2742)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	3	0.14
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB2	9	0.14
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	8	0.14
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	9	0.14
(2,2589)	1:62:A:ASN:HB3	1:43:A:TRP:HZ2	9	0.14
(2,2568)	1:60:A:ILE:HG12	1:60:A:ILE:HD13	4	0.14
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	6	0.14
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	9	0.14
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	10	0.14
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	3	0.14
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	6	0.14
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	9	0.14
(2,2538)	1:58:A:SER:HB2	1:55:A:ASN:HB2	8	0.14
(2,2532)	1:57:A:GLY:HA2	1:56:A:ILE:HG13	9	0.14
(2,2496)	1:51:A:LEU:HB2	1:51:A:LEU:HD12	10	0.14
(2,2478)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	7	0.14
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	6	0.14
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	7	0.14
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	3	0.14
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	9	0.14
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	10	0.14
(2,2387)	1:39:A:VAL:H	1:38:A:ASN:HB3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2381)	1:37:A:VAL:HA	1:37:A:VAL:HG23	6	0.14
(2,2345)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	4	0.14
(2,2329)	1:33:A:LYS:HB3	1:33:A:LYS:HE3	3	0.14
(2,2328)	1:33:A:LYS:HB3	1:33:A:LYS:HD2	7	0.14
(2,2285)	1:28:A:ILE:HA	1:31:A:LEU:HD22	9	0.14
(2,2282)	1:27:A:LYS:HG3	1:27:A:LYS:H	6	0.14
(2,2258)	1:25:A:GLU:HG2	1:48:A:ALA:HB1	10	0.14
(2,2251)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	7	0.14
(2,2244)	1:24:A:THR:HG22	1:24:A:THR:HA	10	0.14
(2,2229)	1:23:A:VAL:HG21	1:16:A:LEU:HG	2	0.14
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG23	4	0.14
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG13	6	0.14
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG12	7	0.14
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG12	10	0.14
(2,2149)	1:15:A:ILE:HD12	1:15:A:ILE:H	10	0.14
(2,2130)	1:14:A:LEU:HD12	2:101:B:MET:HG3	3	0.14
(2,2073)	1:7:A:LEU:HD11	1:7:A:LEU:H	8	0.14
(2,2054)	1:5:A:SER:H	1:4:A:VAL:HG13	4	0.14
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG23	3	0.14
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG21	6	0.14
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG23	10	0.14
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG11	2	0.14
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG12	10	0.14
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB3	8	0.14
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG2	2	0.14
(2,1993)	2:161:B:LYS:HE2	2:161:B:LYS:HG2	8	0.14
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG11	6	0.14
(2,1944)	2:154:B:VAL:HG12	2:154:B:VAL:HA	1	0.14
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD3	2	0.14
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	1	0.14
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	9	0.14
(2,1678)	2:110:B:ALA:HB2	2:118:B:PRO:HA	9	0.14
(2,1673)	2:117:B:SER:HA	2:117:B:SER:HB2	3	0.14
(2,1673)	2:117:B:SER:HA	2:117:B:SER:HB2	8	0.14
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG21	2	0.14
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG22	10	0.14
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG22	4	0.14
(2,1590)	1:60:A:ILE:HA	1:60:A:ILE:HG23	9	0.14
(2,1545)	1:53:A:ASN:HA	1:53:A:ASN:HB3	9	0.14
(2,1536)	1:51:A:LEU:HD21	1:51:A:LEU:HG	6	0.14
(2,1465)	1:37:A:VAL:HG23	1:4:A:VAL:HG11	2	0.14
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1392)	1:24:A:THR:HG22	1:24:A:THR:HA	6	0.14
(2,1392)	1:24:A:THR:HG22	1:24:A:THR:HA	8	0.14
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	8	0.14
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB1	3	0.14
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG12	5	0.14
(2,1240)	2:165:B:VAL:HB	2:166:B:PRO:HD2	4	0.14
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD13	2	0.14
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD12	8	0.14
(2,1187)	2:157:B:GLN:HA	2:157:B:GLN:HB3	9	0.14
(2,1175)	2:154:B:VAL:HG22	2:154:B:VAL:HA	5	0.14
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	2	0.14
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	3	0.14
(2,1105)	2:143:B:ILE:HG23	2:143:B:ILE:HD13	1	0.14
(2,1084)	2:103:B:TYR:HB2	2:142:B:VAL:HG13	5	0.14
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG12	1	0.14
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG13	6	0.14
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG11	8	0.14
(2,1063)	2:139:B:LEU:HD21	2:103:B:TYR:HE1	9	0.14
(2,1048)	2:138:B:ARG:HA	2:138:B:ARG:HD3	8	0.14
(2,1034)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	2	0.14
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	1	0.14
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	7	0.14
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB3	1	0.14
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB2	3	0.14
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB2	8	0.14
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG2	5	0.14
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG2	6	0.14
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	1	0.14
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	2	0.14
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	6	0.14
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	10	0.14
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB2	4	0.14
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB2	5	0.14
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB2	8	0.14
(2,800)	2:105:B:ALA:HB3	2:101:B:MET:HG2	4	0.14
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG13	4	0.14
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG11	6	0.14
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG13	10	0.14
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG13	2	0.14
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG13	7	0.14
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG11	8	0.14
(2,726)	1:58:A:SER:HB3	1:58:A:SER:HA	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,708)	1:54:A:VAL:HA	1:54:A:VAL:HG12	7	0.14
(2,682)	1:50:A:ALA:HB3	1:46:A:LEU:HB3	3	0.14
(2,682)	1:50:A:ALA:HB2	1:46:A:LEU:HB2	8	0.14
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	3	0.14
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD13	8	0.14
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	7	0.14
(2,641)	1:43:A:TRP:HA	1:42:A:PHE:HD1	10	0.14
(2,628)	1:40:A:GLU:HG2	1:41:A:PRO:HD3	4	0.14
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	1	0.14
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	2	0.14
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	5	0.14
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	9	0.14
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	10	0.14
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	9	0.14
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	10	0.14
(2,605)	1:43:A:TRP:HE1	1:39:A:VAL:HG13	7	0.14
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG22	3	0.14
(2,588)	1:37:A:VAL:HG21	2:112:B:LEU:HG	3	0.14
(2,588)	1:37:A:VAL:HG23	2:112:B:LEU:HG	4	0.14
(2,588)	1:37:A:VAL:HG22	2:112:B:LEU:HG	6	0.14
(2,566)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	4	0.14
(2,496)	1:25:A:GLU:HB2	1:25:A:GLU:HG3	9	0.14
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG21	4	0.14
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG12	10	0.14
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG21	4	0.14
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG12	10	0.14
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	2	0.14
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	6	0.14
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE2	8	0.14
(2,372)	1:4:A:VAL:HA	1:7:A:LEU:HD21	6	0.14
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	7	0.14
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	7	0.14
(2,341)	1:1:A:MET:HG2	1:7:A:LEU:HD22	7	0.14
(2,339)	1:1:A:MET:HB2	1:1:A:MET:HA	4	0.14
(2,299)	2:146:B:LEU:H	2:146:B:LEU:HD22	8	0.14
(2,267)	2:134:B:ALA:H	2:133:B:GLU:HB3	8	0.14
(2,161)	1:64:A:GLY:H	1:64:A:GLY:HA3	1	0.14
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD11	2	0.14
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD13	3	0.14
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD11	7	0.14
(2,110)	1:39:A:VAL:H	1:41:A:PRO:HD3	1	0.14
(2,109)	1:39:A:VAL:H	1:38:A:ASN:HB3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD21	8	0.14
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	3	0.14
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	2	0.14
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	6	0.14
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	9	0.14
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	9	0.14
(1,91)	2:144:B:SER:N	2:140:B:ASN:O	2	0.14
(1,87)	2:142:B:VAL:N	2:138:B:ARG:O	9	0.14
(1,75)	2:126:B:ILE:N	2:122:B:ASP:O	3	0.14
(1,75)	2:126:B:ILE:N	2:122:B:ASP:O	7	0.14
(1,55)	2:107:B:TYR:N	2:103:B:TYR:O	8	0.14
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	7	0.14
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	9	0.14
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	10	0.14
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	5	0.14
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	9	0.14
(1,32)	1:31:A:LEU:H	1:27:A:LYS:O	4	0.14
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	9	0.14
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	10	0.14
(1,25)	1:28:A:ILE:N	1:24:A:THR:O	6	0.14
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	4	0.14
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	8	0.14
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	4	0.13
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	8	0.13
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	3	0.13
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	8	0.13
(2,4522)	2:146:B:LEU:HA	2:146:B:LEU:HG	1	0.13
(2,4522)	2:146:B:LEU:HA	2:146:B:LEU:HG	6	0.13
(2,4520)	2:145:B:GLU:HG2	2:145:B:GLU:H	3	0.13
(2,4520)	2:145:B:GLU:HG2	2:145:B:GLU:H	7	0.13
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	5	0.13
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	3	0.13
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	4	0.13
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	5	0.13
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	7	0.13
(2,4458)	2:125:B:LYS:HA	2:125:B:LYS:HB3	4	0.13
(2,4446)	2:120:B:ALA:HA	2:140:B:ASN:HA	3	0.13
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	2	0.13
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	5	0.13
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	10	0.13
(2,4341)	1:41:A:PRO:HA	1:39:A:VAL:H	2	0.13
(2,4341)	1:41:A:PRO:HA	1:39:A:VAL:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	4	0.13
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	3	0.13
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	4	0.13
(2,4247)	1:14:A:LEU:HG	1:14:A:LEU:HA	9	0.13
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	10	0.13
(2,4136)	1:22:A:THR:HA	1:22:A:THR:HB	5	0.13
(2,4136)	1:22:A:THR:HA	1:22:A:THR:HB	9	0.13
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	7	0.13
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	1	0.13
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	2	0.13
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	9	0.13
(2,4046)	1:56:A:ILE:HG12	1:56:A:ILE:HA	4	0.13
(2,4001)	2:164:B:SER:H	2:163:B:ALA:HA	1	0.13
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	7	0.13
(2,3954)	2:143:B:ILE:H	2:107:B:TYR:HE2	8	0.13
(2,3783)	2:108:B:LEU:H	2:108:B:LEU:HG	1	0.13
(2,3728)	1:55:A:ASN:H	1:54:A:VAL:H	4	0.13
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	2	0.13
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	7	0.13
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	4	0.13
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	5	0.13
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	6	0.13
(2,3528)	1:5:A:SER:H	1:3:A:SER:HA	8	0.13
(2,3494)	1:7:A:LEU:HD12	2:155:B:ILE:HG23	6	0.13
(2,3387)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	9	0.13
(2,3340)	1:15:A:ILE:HD11	2:127:B:LEU:HB3	10	0.13
(2,3308)	1:4:A:VAL:HG12	2:112:B:LEU:HD23	4	0.13
(2,3307)	1:4:A:VAL:HG11	2:112:B:LEU:HA	4	0.13
(2,3268)	2:165:B:VAL:HB	2:165:B:VAL:HG13	7	0.13
(2,3263)	2:164:B:SER:HA	2:164:B:SER:HB3	1	0.13
(2,3251)	2:162:B:LEU:HA	2:162:B:LEU:HD12	5	0.13
(2,3250)	2:162:B:LEU:HD11	2:162:B:LEU:HG	1	0.13
(2,3250)	2:162:B:LEU:HD11	2:162:B:LEU:HG	9	0.13
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	1	0.13
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	2	0.13
(2,3236)	2:161:B:LYS:HA	2:161:B:LYS:HB3	3	0.13
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB1	6	0.13
(2,3145)	2:151:B:ILE:HG22	2:152:B:GLU:HG2	1	0.13
(2,3086)	2:144:B:SER:HA	2:144:B:SER:HB2	3	0.13
(2,3085)	2:144:B:SER:H	2:144:B:SER:HB2	6	0.13
(2,3049)	2:142:B:VAL:HG12	2:107:B:TYR:HE2	8	0.13
(2,3043)	2:141:B:LYS:HA	2:144:B:SER:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3043)	2:141:B:LYS:HA	2:144:B:SER:H	10	0.13
(2,3011)	2:137:B:ASP:HB2	2:138:B:ARG:HG2	3	0.13
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB1	10	0.13
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD12	3	0.13
(2,2872)	2:125:B:LYS:HD3	2:125:B:LYS:HB2	2	0.13
(2,2862)	2:124:B:LYS:HE2	2:124:B:LYS:HD3	3	0.13
(2,2861)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	2	0.13
(2,2819)	2:120:B:ALA:HA	2:120:B:ALA:HB2	4	0.13
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB1	2	0.13
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB2	3	0.13
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	8	0.13
(2,2767)	2:116:B:SER:H	2:115:B:ASN:HB2	1	0.13
(2,2748)	2:112:B:LEU:H	2:112:B:LEU:HD12	7	0.13
(2,2683)	2:108:B:LEU:HD23	2:104:B:VAL:HB	4	0.13
(2,2647)	2:104:B:VAL:HG22	2:146:B:LEU:HD22	6	0.13
(2,2629)	1:14:A:LEU:HD12	2:101:B:MET:HE1	3	0.13
(2,2602)	1:43:A:TRP:HD1	1:6:A:GLU:HG3	5	0.13
(2,2602)	1:43:A:TRP:HD1	1:6:A:GLU:HG3	9	0.13
(2,2590)	1:62:A:ASN:H	1:62:A:ASN:HB3	1	0.13
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	2	0.13
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	3	0.13
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	4	0.13
(2,2511)	1:54:A:VAL:HG22	1:58:A:SER:HB3	1	0.13
(2,2477)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	5	0.13
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	5	0.13
(2,2473)	1:49:A:LYS:HA	1:49:A:LYS:HB3	9	0.13
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG2	10	0.13
(2,2324)	1:32:A:ILE:HD12	1:31:A:LEU:H	1	0.13
(2,2324)	1:32:A:ILE:HD12	1:31:A:LEU:H	10	0.13
(2,2245)	1:24:A:THR:HG21	1:27:A:LYS:HE3	8	0.13
(2,2244)	1:24:A:THR:HG23	1:24:A:THR:HA	1	0.13
(2,2244)	1:24:A:THR:HG23	1:24:A:THR:HA	7	0.13
(2,2231)	1:23:A:VAL:H	1:23:A:VAL:HG23	9	0.13
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG21	3	0.13
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG12	1	0.13
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG12	2	0.13
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG13	8	0.13
(2,2204)	1:20:A:GLU:HG2	1:19:A:ASP:H	10	0.13
(2,2149)	1:15:A:ILE:HD12	1:15:A:ILE:H	5	0.13
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE2	1	0.13
(2,2138)	1:14:A:LEU:HG	2:101:B:MET:HE1	2	0.13
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG21	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG22	5	0.13
(2,2050)	1:5:A:SER:H	1:4:A:VAL:HG11	3	0.13
(2,2045)	1:4:A:VAL:HA	1:7:A:LEU:HD21	5	0.13
(2,1995)	2:162:B:LEU:HA	2:162:B:LEU:HB3	9	0.13
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	6	0.13
(2,1968)	2:157:B:GLN:HA	2:157:B:GLN:HB3	7	0.13
(2,1967)	2:157:B:GLN:HA	2:157:B:GLN:HG2	9	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG21	2	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG21	3	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG13	4	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG12	5	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG12	7	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG11	8	0.13
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG21	10	0.13
(2,1944)	2:154:B:VAL:HG12	2:154:B:VAL:HA	3	0.13
(2,1944)	2:154:B:VAL:HG12	2:154:B:VAL:HA	4	0.13
(2,1944)	2:154:B:VAL:HG13	2:154:B:VAL:HA	6	0.13
(2,1853)	2:140:B:ASN:HA	2:140:B:ASN:HB2	9	0.13
(2,1851)	2:139:B:LEU:HD12	2:120:B:ALA:HA	6	0.13
(2,1834)	2:138:B:ARG:HG2	2:138:B:ARG:HD3	1	0.13
(2,1820)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	5	0.13
(2,1820)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.13
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	4	0.13
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	6	0.13
(2,1757)	2:125:B:LYS:HD3	2:125:B:LYS:HG2	6	0.13
(2,1757)	2:125:B:LYS:HD3	2:125:B:LYS:HG2	9	0.13
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB3	6	0.13
(2,1709)	2:121:B:LYS:HA	2:121:B:LYS:HD2	7	0.13
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	2	0.13
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	3	0.13
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	7	0.13
(2,1673)	2:117:B:SER:HA	2:117:B:SER:HB2	4	0.13
(2,1567)	1:56:A:ILE:HD12	1:59:A:LEU:HG	5	0.13
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	10	0.13
(2,1392)	1:24:A:THR:HG22	1:24:A:THR:HA	3	0.13
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	6	0.13
(2,1361)	1:20:A:GLU:HA	1:20:A:GLU:HG2	10	0.13
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB2	1	0.13
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD12	6	0.13
(2,1225)	2:162:B:LEU:HB3	2:162:B:LEU:HG	8	0.13
(2,1164)	2:152:B:GLU:HA	2:152:B:GLU:HG2	8	0.13
(2,1153)	2:151:B:ILE:HA	2:151:B:ILE:HD11	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1135)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	4	0.13
(2,1117)	2:145:B:GLU:HA	2:145:B:GLU:HG2	4	0.13
(2,1115)	2:144:B:SER:HA	2:147:B:ASN:HB3	10	0.13
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	2	0.13
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	8	0.13
(2,1081)	2:142:B:VAL:HG12	2:107:B:TYR:HE2	8	0.13
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG13	10	0.13
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB3	1	0.13
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB3	8	0.13
(2,1018)	2:133:B:GLU:HA	2:133:B:GLU:HB3	9	0.13
(2,956)	2:125:B:LYS:HA	2:125:B:LYS:HG2	8	0.13
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	7	0.13
(2,881)	2:116:B:SER:HA	2:116:B:SER:HB3	6	0.13
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB1	1	0.13
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB1	3	0.13
(2,826)	2:108:B:LEU:HD23	2:104:B:VAL:HB	10	0.13
(2,793)	2:104:B:VAL:HG12	2:104:B:VAL:HB	3	0.13
(2,793)	2:104:B:VAL:HG23	2:104:B:VAL:HB	8	0.13
(2,793)	2:104:B:VAL:HG23	2:104:B:VAL:HB	10	0.13
(2,788)	2:104:B:VAL:HA	2:104:B:VAL:HG13	5	0.13
(2,786)	2:104:B:VAL:HA	2:107:B:TYR:HD1	7	0.13
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	3	0.13
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE1	8	0.13
(2,756)	1:65:A:ALA:HB1	1:65:A:ALA:HA	8	0.13
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG11	5	0.13
(2,754)	1:63:A:VAL:HA	1:63:A:VAL:HG13	6	0.13
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	3	0.13
(2,740)	1:59:A:LEU:HD13	1:56:A:ILE:HA	7	0.13
(2,726)	1:58:A:SER:HB3	1:58:A:SER:HA	5	0.13
(2,683)	1:50:A:ALA:HB3	1:54:A:VAL:HG23	2	0.13
(2,683)	1:50:A:ALA:HB2	1:54:A:VAL:HG23	7	0.13
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	5	0.13
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	8	0.13
(2,670)	1:49:A:LYS:HA	1:49:A:LYS:HB3	2	0.13
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	8	0.13
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	3	0.13
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	7	0.13
(2,623)	1:41:A:PRO:HA	1:41:A:PRO:HG3	8	0.13
(2,617)	1:40:A:GLU:HG3	1:40:A:GLU:HA	3	0.13
(2,615)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	1	0.13
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG21	1	0.13
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG21	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,599)	1:39:A:VAL:HA	1:39:A:VAL:HG11	2	0.13
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG22	9	0.13
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG23	10	0.13
(2,588)	1:37:A:VAL:HG21	2:112:B:LEU:HG	1	0.13
(2,588)	1:37:A:VAL:HG23	2:112:B:LEU:HG	7	0.13
(2,571)	1:35:A:ALA:HA	2:126:B:ILE:HG13	9	0.13
(2,560)	1:33:A:LYS:HA	1:33:A:LYS:HG3	9	0.13
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG2	3	0.13
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG3	4	0.13
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG2	6	0.13
(2,515)	1:27:A:LYS:HG2	1:27:A:LYS:HE2	6	0.13
(2,500)	1:26:A:ASP:HA	1:29:A:ASN:HB3	7	0.13
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG23	8	0.13
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG12	10	0.13
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG21	5	0.13
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG23	8	0.13
(2,462)	1:21:A:VAL:HG11	1:16:A:LEU:HG	4	0.13
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE1	10	0.13
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	1	0.13
(2,347)	1:2:A:ALA:HB2	1:7:A:LEU:HB2	3	0.13
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	4	0.13
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	8	0.13
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB2	8	0.13
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	1	0.13
(2,329)	2:164:B:SER:H	2:162:B:LEU:HB3	3	0.13
(2,304)	2:149:B:LYS:H	2:149:B:LYS:HE2	6	0.13
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD12	3	0.13
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG11	8	0.13
(2,157)	1:62:A:ASN:H	1:62:A:ASN:HB3	1	0.13
(2,36)	1:13:A:ALA:H	1:51:A:LEU:HD13	2	0.13
(2,20)	1:8:A:ALA:H	1:7:A:LEU:HD21	4	0.13
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	1	0.13
(2,6)	1:59:A:LEU:H	1:56:A:ILE:O	3	0.13
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	2	0.13
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	4	0.13
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	8	0.13
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	10	0.13
(1,87)	2:142:B:VAL:N	2:138:B:ARG:O	5	0.13
(1,87)	2:142:B:VAL:N	2:138:B:ARG:O	8	0.13
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	7	0.13
(1,81)	2:129:B:SER:N	2:125:B:LYS:O	7	0.13
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	5	0.13
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	6	0.13
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	7	0.13
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	1	0.13
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	4	0.13
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	8	0.13
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	2	0.13
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	8	0.13
(1,24)	1:27:A:LYS:H	1:24:A:THR:O	1	0.13
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	3	0.13
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	9	0.13
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	10	0.12
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	5	0.12
(2,4531)	2:151:B:ILE:HB	2:150:B:ASN:H	9	0.12
(2,4522)	2:146:B:LEU:HA	2:146:B:LEU:HG	4	0.12
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	2	0.12
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	10	0.12
(2,4512)	2:143:B:ILE:HA	2:146:B:LEU:HG	7	0.12
(2,4509)	2:142:B:VAL:HB	2:143:B:ILE:H	10	0.12
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	4	0.12
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	1	0.12
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	2	0.12
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	6	0.12
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	8	0.12
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	10	0.12
(2,4446)	2:120:B:ALA:HA	2:140:B:ASN:HA	10	0.12
(2,4393)	1:63:A:VAL:HA	1:64:A:GLY:H	8	0.12
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	8	0.12
(2,4282)	1:22:A:THR:HA	1:23:A:VAL:HB	9	0.12
(2,4251)	1:15:A:ILE:HA	2:103:B:TYR:HA	5	0.12
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	2	0.12
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	8	0.12
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	9	0.12
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	3	0.12
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	8	0.12
(2,4046)	1:56:A:ILE:HG12	1:56:A:ILE:HA	1	0.12
(2,3999)	2:160:B:GLY:H	2:162:B:LEU:H	10	0.12
(2,3954)	2:143:B:ILE:H	2:107:B:TYR:HE2	1	0.12
(2,3954)	2:143:B:ILE:H	2:107:B:TYR:HE2	5	0.12
(2,3783)	2:108:B:LEU:H	2:108:B:LEU:HG	3	0.12
(2,3736)	1:58:A:SER:H	1:55:A:ASN:HA	1	0.12
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	8	0.12
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	10	0.12
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	5	0.12
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	8	0.12
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	9	0.12
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	10	0.12
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	2	0.12
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	8	0.12
(2,3498)	2:159:B:ILE:HD12	1:7:A:LEU:HA	2	0.12
(2,3489)	2:152:B:GLU:HG3	1:7:A:LEU:HG	4	0.12
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	8	0.12
(2,3430)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	9	0.12
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	8	0.12
(2,3400)	1:59:A:LEU:HD12	2:159:B:ILE:HG22	10	0.12
(2,3388)	1:37:A:VAL:HG21	2:112:B:LEU:HD23	1	0.12
(2,3388)	1:37:A:VAL:HG21	2:112:B:LEU:HD22	3	0.12
(2,3387)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	4	0.12
(2,3386)	1:37:A:VAL:HG11	2:109:B:LEU:HD13	8	0.12
(2,3317)	1:8:A:ALA:HB1	2:109:B:LEU:HG	1	0.12
(2,3302)	1:4:A:VAL:HB	2:112:B:LEU:HD22	2	0.12
(2,3273)	2:165:B:VAL:HA	2:165:B:VAL:HG12	3	0.12
(2,3255)	2:162:B:LEU:HD21	2:104:B:VAL:HB	5	0.12
(2,3248)	2:162:B:LEU:HB2	2:162:B:LEU:HD12	3	0.12
(2,3248)	2:162:B:LEU:HB3	2:162:B:LEU:HD21	5	0.12
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	6	0.12
(2,3234)	2:159:B:ILE:HG23	1:61:A:CYS:H	5	0.12
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG3	1	0.12
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG3	6	0.12
(2,3211)	2:157:B:GLN:H	2:157:B:GLN:HG2	10	0.12
(2,3168)	2:154:B:VAL:HG22	2:154:B:VAL:HA	5	0.12
(2,3139)	2:151:B:ILE:HB	2:151:B:ILE:HD13	3	0.12
(2,3104)	2:146:B:LEU:HD22	2:146:B:LEU:HG	6	0.12
(2,3074)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	9	0.12
(2,3011)	2:137:B:ASP:HB2	2:138:B:ARG:HG2	10	0.12
(2,2981)	2:134:B:ALA:H	2:134:B:ALA:HB1	4	0.12
(2,2979)	2:134:B:ALA:HB2	2:103:B:TYR:HD1	1	0.12
(2,2965)	2:132:B:ILE:HG21	2:133:B:GLU:HB2	7	0.12
(2,2959)	2:132:B:ILE:HG21	2:133:B:GLU:HB2	7	0.12
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD12	7	0.12
(2,2842)	2:123:B:ILE:HG23	2:139:B:LEU:H	7	0.12
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB2	10	0.12
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2730)	2:108:B:LEU:HA	2:111:B:ALA:HB3	3	0.12
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB2	4	0.12
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB3	10	0.12
(2,2714)	2:110:B:ALA:HB3	2:123:B:ILE:H	6	0.12
(2,2654)	2:105:B:ALA:HB3	2:162:B:LEU:HD23	7	0.12
(2,2647)	2:104:B:VAL:HG22	2:146:B:LEU:HD22	7	0.12
(2,2629)	1:14:A:LEU:HD12	2:101:B:MET:HE2	7	0.12
(2,2601)	1:11:A:TYR:HE1	2:108:B:LEU:HD21	1	0.12
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	1	0.12
(2,2568)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	5	0.12
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	5	0.12
(2,2559)	1:59:A:LEU:HA	1:59:A:LEU:HD21	5	0.12
(2,2514)	1:54:A:VAL:HG22	1:58:A:SER:HB2	8	0.12
(2,2482)	1:50:A:ALA:HB1	1:54:A:VAL:HG22	5	0.12
(2,2477)	1:49:A:LYS:HD3	1:49:A:LYS:HE2	2	0.12
(2,2474)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	6	0.12
(2,2417)	1:40:A:GLU:HG3	1:40:A:GLU:HA	3	0.12
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG2	5	0.12
(2,2415)	1:43:A:TRP:HE1	1:40:A:GLU:HG2	8	0.12
(2,2398)	1:8:A:ALA:HB2	1:39:A:VAL:HG22	9	0.12
(2,2335)	1:33:A:LYS:HA	1:33:A:LYS:HG2	1	0.12
(2,2335)	1:33:A:LYS:HA	1:33:A:LYS:HG3	10	0.12
(2,2330)	1:33:A:LYS:HA	1:33:A:LYS:HB3	8	0.12
(2,2318)	1:32:A:ILE:HD13	1:9:A:CYS:H	6	0.12
(2,2259)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	2	0.12
(2,2259)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	8	0.12
(2,2244)	1:24:A:THR:HG21	1:24:A:THR:HA	9	0.12
(2,2243)	1:24:A:THR:H	1:24:A:THR:HG22	7	0.12
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG22	7	0.12
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG22	8	0.12
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG12	4	0.12
(2,2142)	1:15:A:ILE:HD13	1:15:A:ILE:HA	7	0.12
(2,2057)	1:4:A:VAL:HG13	2:112:B:LEU:HB3	9	0.12
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG21	4	0.12
(2,2053)	1:4:A:VAL:H	1:4:A:VAL:HG22	5	0.12
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG21	4	0.12
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG21	9	0.12
(2,2034)	1:2:A:ALA:HB3	1:6:A:GLU:H	9	0.12
(2,2008)	2:165:B:VAL:HA	2:165:B:VAL:HG11	6	0.12
(2,2007)	2:165:B:VAL:HA	2:166:B:PRO:HD2	7	0.12
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB3	3	0.12
(2,1990)	2:161:B:LYS:HA	2:161:B:LYS:HB3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1966)	2:156:B:ALA:HA	2:156:B:ALA:HB3	8	0.12
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG13	1	0.12
(2,1951)	2:154:B:VAL:HB	2:154:B:VAL:HG12	9	0.12
(2,1944)	2:154:B:VAL:HG13	2:154:B:VAL:HA	8	0.12
(2,1932)	2:152:B:GLU:HB2	2:152:B:GLU:HG3	3	0.12
(2,1881)	2:144:B:SER:HA	2:147:B:ASN:HB3	6	0.12
(2,1834)	2:138:B:ARG:HG2	2:138:B:ARG:HD3	10	0.12
(2,1820)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	6	0.12
(2,1814)	2:133:B:GLU:HA	2:133:B:GLU:HG2	2	0.12
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	2	0.12
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	5	0.12
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	8	0.12
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	10	0.12
(2,1757)	2:125:B:LYS:HD3	2:125:B:LYS:HG2	8	0.12
(2,1746)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	4	0.12
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB3	10	0.12
(2,1720)	2:122:B:ASP:HA	2:125:B:LYS:HD2	1	0.12
(2,1709)	2:121:B:LYS:HA	2:121:B:LYS:HD2	8	0.12
(2,1665)	1:4:A:VAL:HB	2:112:B:LEU:HD22	2	0.12
(2,1610)	1:65:A:ALA:HB1	1:65:A:ALA:HA	8	0.12
(2,1595)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	7	0.12
(2,1595)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	8	0.12
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG22	8	0.12
(2,1568)	1:58:A:SER:HB3	1:58:A:SER:HA	5	0.12
(2,1568)	1:58:A:SER:HB3	1:58:A:SER:HA	8	0.12
(2,1567)	1:56:A:ILE:HD11	1:59:A:LEU:HG	10	0.12
(2,1556)	1:55:A:ASN:HA	1:55:A:ASN:HB2	7	0.12
(2,1556)	1:55:A:ASN:HA	1:55:A:ASN:HB2	9	0.12
(2,1545)	1:53:A:ASN:HA	1:53:A:ASN:HB2	8	0.12
(2,1442)	1:33:A:LYS:HA	1:33:A:LYS:HG3	9	0.12
(2,1402)	1:26:A:ASP:HB2	1:26:A:ASP:HA	9	0.12
(2,1392)	1:24:A:THR:HG22	1:24:A:THR:HA	10	0.12
(2,1381)	1:23:A:VAL:HG11	1:48:A:ALA:HB1	7	0.12
(2,1373)	1:22:A:THR:HG21	1:21:A:VAL:HB	4	0.12
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	2	0.12
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	7	0.12
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	1	0.12
(2,1319)	1:10:A:ILE:HG21	1:14:A:LEU:HG	6	0.12
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	6	0.12
(2,1198)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	3	0.12
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	3	0.12
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1152)	2:151:B:ILE:HD12	2:151:B:ILE:HG13	9	0.12
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	6	0.12
(2,1105)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	9	0.12
(2,1087)	2:142:B:VAL:HA	2:142:B:VAL:HG22	3	0.12
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG12	9	0.12
(2,1063)	2:139:B:LEU:HD21	2:103:B:TYR:HE1	1	0.12
(2,1060)	2:139:B:LEU:HD23	2:124:B:LYS:HD2	4	0.12
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB2	7	0.12
(2,1033)	2:134:B:ALA:HB3	2:139:B:LEU:HD22	7	0.12
(2,1021)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	5	0.12
(2,1017)	2:132:B:ILE:HG21	2:133:B:GLU:HB2	7	0.12
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB3	7	0.12
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB3	9	0.12
(2,942)	2:124:B:LYS:HA	2:124:B:LYS:HG2	7	0.12
(2,890)	2:118:B:PRO:HA	2:118:B:PRO:HG3	8	0.12
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB2	6	0.12
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB1	7	0.12
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB2	9	0.12
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB3	2	0.12
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB2	7	0.12
(2,852)	2:110:B:ALA:HA	2:110:B:ALA:HB3	2	0.12
(2,851)	2:107:B:TYR:HA	2:110:B:ALA:HB2	5	0.12
(2,793)	2:104:B:VAL:HG12	2:104:B:VAL:HB	2	0.12
(2,793)	2:104:B:VAL:HG12	2:104:B:VAL:HB	4	0.12
(2,793)	2:104:B:VAL:HG12	2:104:B:VAL:HB	6	0.12
(2,786)	2:104:B:VAL:HA	2:107:B:TYR:HD2	8	0.12
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	2	0.12
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	6	0.12
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	4	0.12
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	6	0.12
(2,735)	1:59:A:LEU:HA	1:59:A:LEU:HD21	9	0.12
(2,726)	1:58:A:SER:HB3	1:58:A:SER:HA	3	0.12
(2,725)	1:57:A:GLY:HA2	1:60:A:ILE:HB	3	0.12
(2,719)	1:56:A:ILE:HD13	1:17:A:HIS:HD2	10	0.12
(2,678)	1:49:A:LYS:HA	1:49:A:LYS:HD2	9	0.12
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD12	2	0.12
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD13	4	0.12
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD11	10	0.12
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	2	0.12
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	6	0.12
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG13	2	0.12
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG21	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG13	9	0.12
(2,599)	1:39:A:VAL:HA	1:39:A:VAL:HG13	7	0.12
(2,598)	1:38:A:ASN:HB2	1:38:A:ASN:HA	8	0.12
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG21	4	0.12
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB3	7	0.12
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB3	7	0.12
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG21	5	0.12
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG21	9	0.12
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG21	4	0.12
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG23	8	0.12
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG21	9	0.12
(2,431)	1:15:A:ILE:HG23	2:105:B:ALA:HB2	4	0.12
(2,427)	1:15:A:ILE:HG22	2:127:B:LEU:HG	6	0.12
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	3	0.12
(2,347)	1:2:A:ALA:HB1	1:7:A:LEU:HB2	2	0.12
(2,347)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	5	0.12
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB2	4	0.12
(2,344)	1:2:A:ALA:HB1	1:7:A:LEU:HB2	2	0.12
(2,344)	1:2:A:ALA:HB2	1:7:A:LEU:HB2	3	0.12
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	4	0.12
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	5	0.12
(2,344)	1:2:A:ALA:HB3	1:7:A:LEU:HB2	8	0.12
(2,328)	2:163:B:ALA:H	2:162:B:LEU:HB3	7	0.12
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD12	7	0.12
(2,230)	2:121:B:LYS:H	2:119:B:SER:HB2	4	0.12
(2,220)	2:119:B:SER:H	2:119:B:SER:HB3	5	0.12
(2,214)	2:117:B:SER:H	2:117:B:SER:HB3	4	0.12
(2,213)	2:116:B:SER:H	2:117:B:SER:HB3	5	0.12
(2,135)	1:51:A:LEU:H	1:51:A:LEU:HD13	5	0.12
(2,72)	1:27:A:LYS:H	1:28:A:ILE:HD11	1	0.12
(2,72)	1:27:A:LYS:H	1:28:A:ILE:HD11	2	0.12
(2,62)	1:24:A:THR:H	1:24:A:THR:HG23	9	0.12
(2,41)	1:15:A:ILE:H	1:31:A:LEU:HD21	3	0.12
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	3	0.12
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	6	0.12
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	7	0.12
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	9	0.12
(2,4)	1:37:A:VAL:H	1:32:A:ILE:O	3	0.12
(1,99)	2:155:B:ILE:N	2:151:B:ILE:O	1	0.12
(1,99)	2:155:B:ILE:N	2:151:B:ILE:O	9	0.12
(1,91)	2:144:B:SER:N	2:140:B:ASN:O	5	0.12
(1,87)	2:142:B:VAL:N	2:138:B:ARG:O	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	2:142:B:VAL:N	2:138:B:ARG:O	6	0.12
(1,87)	2:142:B:VAL:N	2:138:B:ARG:O	7	0.12
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	5	0.12
(1,81)	2:129:B:SER:N	2:125:B:LYS:O	5	0.12
(1,73)	2:125:B:LYS:N	2:121:B:LYS:O	3	0.12
(1,61)	2:110:B:ALA:N	2:106:B:SER:O	1	0.12
(1,55)	2:107:B:TYR:N	2:103:B:TYR:O	1	0.12
(1,55)	2:107:B:TYR:N	2:103:B:TYR:O	5	0.12
(1,55)	2:107:B:TYR:N	2:103:B:TYR:O	9	0.12
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	2	0.12
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	4	0.12
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	1	0.12
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	4	0.12
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	8	0.12
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	2	0.12
(1,32)	1:31:A:LEU:H	1:27:A:LYS:O	1	0.12
(1,32)	1:31:A:LEU:H	1:27:A:LYS:O	3	0.12
(1,13)	1:13:A:ALA:N	1:9:A:CYS:O	4	0.12
(1,13)	1:13:A:ALA:N	1:9:A:CYS:O	8	0.12
(1,13)	1:13:A:ALA:N	1:9:A:CYS:O	9	0.12
(1,6)	1:9:A:CYS:H	1:5:A:SER:O	6	0.12
(2,4570)	1:14:A:LEU:HG	2:159:B:ILE:HA	3	0.11
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	1	0.11
(2,4532)	2:151:B:ILE:HD11	2:107:B:TYR:HE1	8	0.11
(2,4522)	2:146:B:LEU:HA	2:146:B:LEU:HG	3	0.11
(2,4522)	2:146:B:LEU:HA	2:146:B:LEU:HG	10	0.11
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	1	0.11
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	3	0.11
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	4	0.11
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	7	0.11
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	8	0.11
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	9	0.11
(2,4512)	2:143:B:ILE:HA	2:146:B:LEU:HG	8	0.11
(2,4512)	2:143:B:ILE:HA	2:146:B:LEU:HG	9	0.11
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	3	0.11
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	6	0.11
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	7	0.11
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	8	0.11
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	10	0.11
(2,4495)	2:139:B:LEU:H	2:138:B:ARG:HA	9	0.11
(2,4393)	1:63:A:VAL:HA	1:64:A:GLY:H	6	0.11
(2,4393)	1:63:A:VAL:HA	1:64:A:GLY:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4360)	1:52:A:ALA:HA	1:23:A:VAL:HG13	3	0.11
(2,4345)	1:43:A:TRP:HA	1:46:A:LEU:HG	7	0.11
(2,4341)	1:41:A:PRO:HA	1:39:A:VAL:H	1	0.11
(2,4341)	1:41:A:PRO:HA	1:39:A:VAL:H	10	0.11
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	3	0.11
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	5	0.11
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	6	0.11
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	7	0.11
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	8	0.11
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	10	0.11
(2,4212)	1:3:A:SER:HA	1:4:A:VAL:HB	3	0.11
(2,4173)	2:105:B:ALA:HA	2:108:B:LEU:HD22	3	0.11
(2,4150)	1:39:A:VAL:HB	1:5:A:SER:HA	9	0.11
(2,4136)	1:22:A:THR:HA	1:22:A:THR:HB	7	0.11
(2,4098)	2:138:B:ARG:HA	2:138:B:ARG:HG2	5	0.11
(2,4046)	1:56:A:ILE:HG12	1:56:A:ILE:HA	8	0.11
(2,4039)	1:46:A:LEU:HA	1:46:A:LEU:HB3	3	0.11
(2,4017)	1:15:A:ILE:HA	2:132:B:ILE:HB	9	0.11
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	9	0.11
(2,3783)	2:108:B:LEU:H	2:108:B:LEU:HG	4	0.11
(2,3783)	2:108:B:LEU:H	2:108:B:LEU:HG	10	0.11
(2,3755)	1:65:A:ALA:H	1:66:A:GLY:H	4	0.11
(2,3745)	1:61:A:CYS:H	1:62:A:ASN:HA	6	0.11
(2,3745)	1:61:A:CYS:H	1:62:A:ASN:HA	9	0.11
(2,3736)	1:58:A:SER:H	1:55:A:ASN:HA	7	0.11
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	5	0.11
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	6	0.11
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	7	0.11
(2,3731)	1:57:A:GLY:H	1:58:A:SER:HA	9	0.11
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	2	0.11
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	4	0.11
(2,3668)	1:37:A:VAL:H	1:37:A:VAL:HB	6	0.11
(2,3565)	1:14:A:LEU:H	1:14:A:LEU:HB3	3	0.11
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	7	0.11
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	9	0.11
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	10	0.11
(2,3413)	2:101:B:MET:HE1	1:14:A:LEU:HB2	6	0.11
(2,3387)	1:37:A:VAL:HG12	2:113:B:GLY:HA2	8	0.11
(2,3371)	1:34:A:ALA:HB3	2:126:B:ILE:HG13	7	0.11
(2,3371)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	8	0.11
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	2	0.11
(2,3274)	2:165:B:VAL:HG13	2:166:B:PRO:HD2	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3243)	2:162:B:LEU:HB3	2:162:B:LEU:HG	8	0.11
(2,3236)	2:161:B:LYS:HA	2:161:B:LYS:HB3	4	0.11
(2,3234)	2:159:B:ILE:HG21	1:61:A:CYS:H	10	0.11
(2,3211)	2:157:B:GLN:H	2:157:B:GLN:HG2	7	0.11
(2,3141)	2:151:B:ILE:HA	2:151:B:ILE:HD11	4	0.11
(2,3074)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	6	0.11
(2,3074)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	7	0.11
(2,3052)	2:103:B:TYR:HB2	2:142:B:VAL:HG12	2	0.11
(2,3010)	2:138:B:ARG:HG3	2:135:B:ASP:H	8	0.11
(2,3007)	2:138:B:ARG:HA	2:138:B:ARG:HD3	8	0.11
(2,3004)	2:138:B:ARG:HB3	2:138:B:ARG:HD2	1	0.11
(2,2980)	2:134:B:ALA:HB2	2:135:B:ASP:H	3	0.11
(2,2980)	2:134:B:ALA:HB2	2:135:B:ASP:H	7	0.11
(2,2980)	2:134:B:ALA:HB2	2:135:B:ASP:H	9	0.11
(2,2916)	2:128:B:ASP:HB2	2:124:B:LYS:HB3	10	0.11
(2,2885)	2:126:B:ILE:H	2:126:B:ILE:HD12	5	0.11
(2,2861)	2:124:B:LYS:HE3	2:124:B:LYS:HB3	3	0.11
(2,2851)	2:123:B:ILE:HG21	2:126:B:ILE:H	9	0.11
(2,2822)	2:120:B:ALA:HB3	2:140:B:ASN:H	10	0.11
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB2	1	0.11
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB1	9	0.11
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	1	0.11
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	2	0.11
(2,2730)	2:108:B:LEU:HA	2:111:B:ALA:HB2	4	0.11
(2,2730)	2:108:B:LEU:HA	2:111:B:ALA:HB2	5	0.11
(2,2730)	2:108:B:LEU:HA	2:111:B:ALA:HB2	8	0.11
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB2	6	0.11
(2,2727)	2:115:B:ASN:H	2:111:B:ALA:HB3	8	0.11
(2,2727)	2:115:B:ASN:H	2:111:B:ALA:HB3	9	0.11
(2,2720)	2:110:B:ALA:H	2:110:B:ALA:HB3	4	0.11
(2,2596)	1:65:A:ALA:H	1:65:A:ALA:HB1	2	0.11
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	10	0.11
(2,2561)	1:59:A:LEU:HD13	1:56:A:ILE:HA	7	0.11
(2,2559)	1:59:A:LEU:HA	1:59:A:LEU:HD21	10	0.11
(2,2557)	1:59:A:LEU:HD13	1:56:A:ILE:HA	7	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG22	1	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG12	2	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG12	3	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG21	4	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG12	7	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG23	9	0.11
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2482)	1:50:A:ALA:HB3	1:54:A:VAL:HG22	6	0.11
(2,2476)	1:49:A:LYS:HA	1:49:A:LYS:HD2	7	0.11
(2,2458)	1:46:A:LEU:HD22	1:42:A:PHE:HD1	8	0.11
(2,2424)	1:41:A:PRO:HB3	1:41:A:PRO:HG3	4	0.11
(2,2419)	1:41:A:PRO:HA	1:41:A:PRO:HG3	6	0.11
(2,2388)	1:37:A:VAL:HG22	1:38:A:ASN:HB3	9	0.11
(2,2375)	1:37:A:VAL:HB	1:37:A:VAL:HG12	3	0.11
(2,2345)	1:34:A:ALA:HB3	2:126:B:ILE:HG13	7	0.11
(2,2345)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	8	0.11
(2,2335)	1:33:A:LYS:HA	1:33:A:LYS:HG3	5	0.11
(2,2335)	1:33:A:LYS:HA	1:33:A:LYS:HG2	7	0.11
(2,2329)	1:33:A:LYS:HB2	1:33:A:LYS:HE2	4	0.11
(2,2324)	1:32:A:ILE:HD13	1:31:A:LEU:H	9	0.11
(2,2259)	1:25:A:GLU:HB3	1:25:A:GLU:HG2	3	0.11
(2,2229)	1:23:A:VAL:HG22	1:16:A:LEU:HG	10	0.11
(2,2213)	1:21:A:VAL:HB	1:21:A:VAL:HG13	9	0.11
(2,2206)	1:20:A:GLU:H	1:20:A:GLU:HG2	8	0.11
(2,2084)	1:39:A:VAL:HG21	1:9:A:CYS:HA	2	0.11
(2,2084)	1:39:A:VAL:HG21	1:9:A:CYS:HA	6	0.11
(2,2082)	1:8:A:ALA:HB3	1:5:A:SER:HA	1	0.11
(2,2082)	1:8:A:ALA:HB3	1:5:A:SER:HA	9	0.11
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG22	1	0.11
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG23	7	0.11
(2,2006)	2:164:B:SER:HA	2:164:B:SER:HB3	5	0.11
(2,1937)	2:153:B:ASP:HA	2:153:B:ASP:HB3	6	0.11
(2,1931)	2:152:B:GLU:HA	2:152:B:GLU:HB3	6	0.11
(2,1873)	2:143:B:ILE:HD12	2:142:B:VAL:HG12	6	0.11
(2,1870)	2:143:B:ILE:HD11	2:143:B:ILE:HG12	5	0.11
(2,1870)	2:143:B:ILE:HD11	2:143:B:ILE:HG13	9	0.11
(2,1820)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	7	0.11
(2,1820)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	8	0.11
(2,1820)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	9	0.11
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	1	0.11
(2,1813)	2:133:B:GLU:HA	2:133:B:GLU:HB3	7	0.11
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB3	5	0.11
(2,1709)	2:121:B:LYS:HA	2:121:B:LYS:HD2	3	0.11
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	6	0.11
(2,1705)	2:120:B:ALA:HA	2:120:B:ALA:HB3	10	0.11
(2,1673)	2:117:B:SER:HA	2:117:B:SER:HB2	9	0.11
(2,1673)	2:117:B:SER:HA	2:117:B:SER:HB2	10	0.11
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG21	4	0.11
(2,1594)	1:60:A:ILE:HD11	1:60:A:ILE:HG22	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1587)	1:59:A:LEU:HA	1:59:A:LEU:HD21	5	0.11
(2,1574)	1:59:A:LEU:HA	1:62:A:ASN:HB2	4	0.11
(2,1574)	1:59:A:LEU:HA	1:62:A:ASN:HB2	6	0.11
(2,1568)	1:58:A:SER:HB3	1:58:A:SER:HA	3	0.11
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	3	0.11
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	4	0.11
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	9	0.11
(2,1530)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	7	0.11
(2,1485)	1:39:A:VAL:HG12	1:43:A:TRP:HA	1	0.11
(2,1485)	1:39:A:VAL:HG12	1:43:A:TRP:HA	10	0.11
(2,1399)	1:25:A:GLU:HB2	1:48:A:ALA:HB3	3	0.11
(2,1392)	1:24:A:THR:HG23	1:24:A:THR:HA	1	0.11
(2,1392)	1:24:A:THR:HG23	1:24:A:THR:HA	7	0.11
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	1	0.11
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	3	0.11
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	4	0.11
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	10	0.11
(2,1370)	1:19:A:ASP:HB3	1:21:A:VAL:HG12	2	0.11
(2,1370)	1:19:A:ASP:HB3	1:21:A:VAL:HG12	4	0.11
(2,1361)	1:20:A:GLU:HA	1:20:A:GLU:HG2	9	0.11
(2,1274)	1:2:A:ALA:HA	1:2:A:ALA:HB2	5	0.11
(2,1245)	2:165:B:VAL:HA	2:165:B:VAL:HG12	3	0.11
(2,1243)	2:165:B:VAL:HG13	2:166:B:PRO:HD2	9	0.11
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD13	3	0.11
(2,1220)	2:161:B:LYS:HA	2:161:B:LYS:HB3	9	0.11
(2,1198)	2:156:B:ALA:HB3	2:157:B:GLN:HG3	2	0.11
(2,1180)	2:155:B:ILE:HG21	2:155:B:ILE:HG12	6	0.11
(2,1151)	2:151:B:ILE:HB	2:151:B:ILE:HD13	3	0.11
(2,1105)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	6	0.11
(2,1105)	2:143:B:ILE:HG21	2:143:B:ILE:HD13	7	0.11
(2,1100)	2:143:B:ILE:HD11	2:123:B:ILE:HA	6	0.11
(2,1100)	2:143:B:ILE:HD13	2:123:B:ILE:HA	8	0.11
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG12	3	0.11
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG13	5	0.11
(2,1080)	2:142:B:VAL:HB	2:142:B:VAL:HG12	7	0.11
(2,1043)	2:137:B:ASP:HA	2:137:B:ASP:HB3	2	0.11
(2,1038)	2:136:B:ASP:HA	2:136:B:ASP:HB3	2	0.11
(2,1038)	2:136:B:ASP:HA	2:136:B:ASP:HB2	8	0.11
(2,1021)	2:133:B:GLU:HB2	2:133:B:GLU:HG3	6	0.11
(2,1021)	2:133:B:GLU:HB3	2:133:B:GLU:HG2	10	0.11
(2,989)	2:125:B:LYS:HA	2:128:B:ASP:HB3	2	0.11
(2,956)	2:125:B:LYS:HA	2:125:B:LYS:HG2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,956)	2:125:B:LYS:HA	2:125:B:LYS:HG2	6	0.11
(2,948)	2:125:B:LYS:HA	2:125:B:LYS:HG2	7	0.11
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB3	1	0.11
(2,857)	2:108:B:LEU:HA	2:111:B:ALA:HB2	2	0.11
(2,793)	2:104:B:VAL:HG11	2:104:B:VAL:HB	1	0.11
(2,793)	2:104:B:VAL:HG11	2:104:B:VAL:HB	9	0.11
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	7	0.11
(2,782)	2:103:B:TYR:HB3	2:103:B:TYR:HD2	9	0.11
(2,776)	1:14:A:LEU:HA	2:101:B:MET:HE2	4	0.11
(2,773)	2:101:B:MET:HE2	2:101:B:MET:HG3	8	0.11
(2,755)	1:63:A:VAL:HB	1:63:A:VAL:HG22	5	0.11
(2,735)	1:59:A:LEU:HA	1:59:A:LEU:HD21	6	0.11
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	2	0.11
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	4	0.11
(2,677)	1:49:A:LYS:HB3	1:49:A:LYS:HD2	9	0.11
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD13	9	0.11
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD21	5	0.11
(2,652)	1:46:A:LEU:HB2	1:46:A:LEU:HD22	10	0.11
(2,612)	1:39:A:VAL:HA	1:39:A:VAL:HG11	2	0.11
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG21	3	0.11
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG12	8	0.11
(2,604)	1:39:A:VAL:HB	1:39:A:VAL:HG21	10	0.11
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG23	2	0.11
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG22	5	0.11
(2,566)	1:34:A:ALA:HB3	2:126:B:ILE:HG13	7	0.11
(2,566)	1:34:A:ALA:HB2	2:126:B:ILE:HG13	8	0.11
(2,557)	1:33:A:LYS:HA	1:33:A:LYS:HB2	9	0.11
(2,554)	1:33:A:LYS:HA	1:33:A:LYS:HB2	9	0.11
(2,552)	1:33:A:LYS:HA	1:33:A:LYS:HG3	2	0.11
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG21	5	0.11
(2,472)	1:23:A:VAL:HA	1:23:A:VAL:HG23	7	0.11
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	3	0.11
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	7	0.11
(2,431)	1:15:A:ILE:HG23	2:105:B:ALA:HB2	2	0.11
(2,431)	1:15:A:ILE:HG23	2:105:B:ALA:HB2	9	0.11
(2,394)	1:10:A:ILE:HG23	1:10:A:ILE:HA	1	0.11
(2,391)	1:10:A:ILE:HG23	2:159:B:ILE:HG12	5	0.11
(2,383)	1:10:A:ILE:HA	1:13:A:ALA:HB1	4	0.11
(2,383)	1:10:A:ILE:HA	1:13:A:ALA:HB1	9	0.11
(2,346)	1:2:A:ALA:HA	1:2:A:ALA:HB2	7	0.11
(2,339)	1:1:A:MET:HB2	1:1:A:MET:HA	10	0.11
(2,267)	2:134:B:ALA:H	2:133:B:GLU:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,267)	2:134:B:ALA:H	2:133:B:GLU:HB3	6	0.11
(2,248)	2:126:B:ILE:H	2:126:B:ILE:HD12	5	0.11
(2,208)	2:115:B:ASN:H	2:111:B:ALA:HB3	8	0.11
(2,208)	2:115:B:ASN:H	2:111:B:ALA:HB3	9	0.11
(2,161)	1:64:A:GLY:H	1:64:A:GLY:HA2	4	0.11
(2,74)	1:27:A:LYS:H	1:29:A:ASN:HB3	6	0.11
(2,62)	1:24:A:THR:H	1:24:A:THR:HG23	4	0.11
(2,62)	1:24:A:THR:H	1:24:A:THR:HG23	5	0.11
(2,62)	1:24:A:THR:H	1:24:A:THR:HG21	8	0.11
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	8	0.11
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	1	0.11
(2,5)	1:59:A:LEU:N	1:56:A:ILE:O	10	0.11
(1,94)	2:145:B:GLU:H	2:141:B:LYS:O	10	0.11
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	6	0.11
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	8	0.11
(1,75)	2:126:B:ILE:N	2:122:B:ASP:O	6	0.11
(1,73)	2:125:B:LYS:N	2:121:B:LYS:O	9	0.11
(1,56)	2:107:B:TYR:H	2:103:B:TYR:O	1	0.11
(1,55)	2:107:B:TYR:N	2:103:B:TYR:O	7	0.11
(1,47)	1:48:A:ALA:N	1:44:A:PRO:O	9	0.11
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	3	0.11
(1,46)	1:47:A:PHE:H	1:43:A:TRP:O	9	0.11
(1,45)	1:47:A:PHE:N	1:43:A:TRP:O	2	0.11
(1,42)	1:45:A:GLY:H	1:41:A:PRO:O	10	0.11
(1,31)	1:31:A:LEU:N	1:27:A:LYS:O	5	0.11
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	4	0.11
(1,19)	1:16:A:LEU:N	1:12:A:SER:O	7	0.11
(1,13)	1:13:A:ALA:N	1:9:A:CYS:O	2	0.11
(1,6)	1:9:A:CYS:H	1:5:A:SER:O	3	0.11
(1,6)	1:9:A:CYS:H	1:5:A:SER:O	5	0.11
(2,4569)	1:10:A:ILE:HB	2:159:B:ILE:HA	3	0.1
(2,4561)	2:162:B:LEU:HG	2:162:B:LEU:H	2	0.1
(2,4514)	2:144:B:SER:H	2:143:B:ILE:HA	6	0.1
(2,4503)	2:140:B:ASN:HA	2:141:B:LYS:H	2	0.1
(2,4338)	1:39:A:VAL:HB	1:38:A:ASN:HA	6	0.1
(2,4323)	1:33:A:LYS:H	1:33:A:LYS:HB2	10	0.1
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	1	0.1
(2,4250)	1:14:A:LEU:HG	1:11:A:TYR:HA	9	0.1
(2,4136)	1:22:A:THR:HA	1:22:A:THR:HB	10	0.1
(2,4119)	2:155:B:ILE:HB	2:152:B:GLU:HA	9	0.1
(2,4104)	2:143:B:ILE:HA	2:146:B:LEU:HG	1	0.1
(2,4039)	1:46:A:LEU:HA	1:46:A:LEU:HB3	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4039)	1:46:A:LEU:HA	1:46:A:LEU:HB3	5	0.1
(2,4039)	1:46:A:LEU:HA	1:46:A:LEU:HB3	7	0.1
(2,4039)	1:46:A:LEU:HA	1:46:A:LEU:HB3	10	0.1
(2,3838)	2:122:B:ASP:H	2:120:B:ALA:H	8	0.1
(2,3728)	1:55:A:ASN:H	1:54:A:VAL:H	1	0.1
(2,3541)	1:9:A:CYS:H	1:10:A:ILE:HB	1	0.1
(2,3528)	1:5:A:SER:H	1:3:A:SER:HA	5	0.1
(2,3435)	1:37:A:VAL:HG13	2:109:B:LEU:HD11	5	0.1
(2,3318)	1:10:A:ILE:HB	2:159:B:ILE:HG13	3	0.1
(2,3212)	2:157:B:GLN:H	2:157:B:GLN:HG3	3	0.1
(2,3193)	2:156:B:ALA:HA	2:156:B:ALA:HB3	8	0.1
(2,3187)	2:155:B:ILE:HG21	2:155:B:ILE:HB	7	0.1
(2,3162)	2:154:B:VAL:HG22	2:154:B:VAL:HA	7	0.1
(2,3141)	2:151:B:ILE:HA	2:151:B:ILE:HD11	9	0.1
(2,3139)	2:151:B:ILE:HB	2:151:B:ILE:HD13	4	0.1
(2,3071)	2:143:B:ILE:HG21	2:143:B:ILE:HG12	3	0.1
(2,3052)	2:103:B:TYR:HB2	2:142:B:VAL:HG11	7	0.1
(2,3020)	2:139:B:LEU:HD22	2:139:B:LEU:HG	8	0.1
(2,2980)	2:134:B:ALA:HB3	2:135:B:ASP:H	2	0.1
(2,2980)	2:134:B:ALA:HB2	2:135:B:ASP:H	8	0.1
(2,2967)	2:133:B:GLU:HA	2:133:B:GLU:HG2	3	0.1
(2,2871)	2:125:B:LYS:H	2:125:B:LYS:HD3	4	0.1
(2,2842)	2:123:B:ILE:HG23	2:139:B:LEU:H	5	0.1
(2,2814)	2:120:B:ALA:H	2:120:B:ALA:HB2	7	0.1
(2,2778)	2:117:B:SER:H	2:117:B:SER:HB3	9	0.1
(2,2728)	2:111:B:ALA:H	2:111:B:ALA:HB2	8	0.1
(2,2706)	1:8:A:ALA:HA	2:109:B:LEU:HD13	7	0.1
(2,2566)	1:60:A:ILE:HD11	1:60:A:ILE:HB	1	0.1
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG23	6	0.1
(2,2512)	1:54:A:VAL:HB	1:54:A:VAL:HG21	8	0.1
(2,2424)	1:41:A:PRO:HB3	1:41:A:PRO:HG3	1	0.1
(2,2424)	1:41:A:PRO:HB3	1:41:A:PRO:HG3	3	0.1
(2,2424)	1:41:A:PRO:HB3	1:41:A:PRO:HG3	6	0.1
(2,2424)	1:41:A:PRO:HB3	1:41:A:PRO:HG3	7	0.1
(2,2424)	1:41:A:PRO:HB3	1:41:A:PRO:HG3	8	0.1
(2,2419)	1:41:A:PRO:HA	1:41:A:PRO:HG3	4	0.1
(2,2378)	1:37:A:VAL:HB	1:37:A:VAL:HG12	3	0.1
(2,2322)	1:32:A:ILE:HD13	1:9:A:CYS:HA	5	0.1
(2,2229)	1:23:A:VAL:HG22	1:16:A:LEU:HG	1	0.1
(2,2217)	1:22:A:THR:HA	1:23:A:VAL:HG23	9	0.1
(2,2149)	1:15:A:ILE:HD12	1:15:A:ILE:H	3	0.1
(2,2082)	1:8:A:ALA:HB3	1:5:A:SER:HA	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2057)	1:4:A:VAL:HG12	2:112:B:LEU:HB3	6	0.1
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG21	2	0.1
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG23	3	0.1
(2,2051)	1:4:A:VAL:HB	1:4:A:VAL:HG21	8	0.1
(2,2045)	1:4:A:VAL:HA	1:7:A:LEU:HD21	2	0.1
(2,2001)	2:162:B:LEU:HD22	2:101:B:MET:HG3	8	0.1
(2,1999)	2:162:B:LEU:HA	2:162:B:LEU:HD13	1	0.1
(2,1999)	2:162:B:LEU:HA	2:162:B:LEU:HD13	7	0.1
(2,1999)	2:162:B:LEU:HA	2:162:B:LEU:HD11	10	0.1
(2,1968)	2:157:B:GLN:HA	2:157:B:GLN:HB3	10	0.1
(2,1905)	2:147:B:ASN:HA	2:147:B:ASN:HB2	6	0.1
(2,1873)	2:143:B:ILE:HD11	2:142:B:VAL:HG12	8	0.1
(2,1870)	2:143:B:ILE:HD11	2:143:B:ILE:HG12	8	0.1
(2,1842)	2:139:B:LEU:HD12	2:120:B:ALA:HA	6	0.1
(2,1826)	2:136:B:ASP:HA	2:136:B:ASP:HB2	7	0.1
(2,1824)	2:134:B:ALA:HB3	2:124:B:LYS:HE2	3	0.1
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB3	1	0.1
(2,1722)	2:122:B:ASP:HA	2:122:B:ASP:HB3	2	0.1
(2,1678)	2:110:B:ALA:HB2	2:118:B:PRO:HA	7	0.1
(2,1641)	2:108:B:LEU:HD21	2:155:B:ILE:HG21	7	0.1
(2,1595)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	9	0.1
(2,1595)	1:60:A:ILE:HG13	1:60:A:ILE:HD12	10	0.1
(2,1587)	1:59:A:LEU:HA	1:59:A:LEU:HD21	10	0.1
(2,1569)	1:58:A:SER:HA	1:61:A:CYS:HB2	4	0.1
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	1	0.1
(2,1533)	1:49:A:LYS:HE2	1:49:A:LYS:HG3	8	0.1
(2,1528)	1:49:A:LYS:HD2	1:49:A:LYS:HE3	1	0.1
(2,1402)	1:26:A:ASP:HB2	1:26:A:ASP:HA	1	0.1
(2,1372)	1:22:A:THR:HB	1:22:A:THR:HG23	8	0.1
(2,1364)	1:20:A:GLU:HB2	1:20:A:GLU:HG3	9	0.1
(2,1361)	1:20:A:GLU:HA	1:20:A:GLU:HG2	4	0.1
(2,1287)	1:4:A:VAL:HB	1:4:A:VAL:HG22	5	0.1
(2,1232)	2:162:B:LEU:HA	2:162:B:LEU:HD11	9	0.1
(2,1135)	2:146:B:LEU:HB3	2:146:B:LEU:HD13	1	0.1
(2,1110)	2:143:B:ILE:HA	2:143:B:ILE:HG21	9	0.1
(2,1038)	2:136:B:ASP:HA	2:136:B:ASP:HB3	1	0.1
(2,949)	2:125:B:LYS:HA	2:128:B:ASP:HB2	6	0.1
(2,854)	2:111:B:ALA:HA	2:111:B:ALA:HB3	9	0.1
(2,852)	2:110:B:ALA:HA	2:110:B:ALA:HB3	8	0.1
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	3	0.1
(2,751)	1:61:A:CYS:HA	1:61:A:CYS:HB2	9	0.1
(2,705)	1:54:A:VAL:HA	1:54:A:VAL:HG13	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,705)	1:54:A:VAL:HA	1:54:A:VAL:HG12	9	0.1
(2,671)	1:49:A:LYS:HA	1:49:A:LYS:HD2	1	0.1
(2,654)	1:46:A:LEU:HA	1:46:A:LEU:HD13	6	0.1
(2,612)	1:39:A:VAL:HA	1:39:A:VAL:HG13	7	0.1
(2,590)	1:37:A:VAL:HA	1:37:A:VAL:HG21	8	0.1
(2,582)	1:37:A:VAL:HA	1:37:A:VAL:HG23	6	0.1
(2,551)	1:32:A:ILE:HD13	1:9:A:CYS:HA	5	0.1
(2,500)	1:26:A:ASP:HA	1:29:A:ASN:HB2	4	0.1
(2,483)	1:23:A:VAL:HA	1:23:A:VAL:HG23	7	0.1
(2,480)	1:23:A:VAL:HA	1:23:A:VAL:HG21	9	0.1
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	5	0.1
(2,458)	1:20:A:GLU:HA	1:20:A:GLU:HG2	8	0.1
(2,431)	1:15:A:ILE:HG23	2:105:B:ALA:HB1	5	0.1
(2,417)	1:14:A:LEU:HG	2:101:B:MET:HE2	7	0.1
(2,257)	2:129:B:SER:H	1:31:A:LEU:HD11	5	0.1
(2,214)	2:117:B:SER:H	2:117:B:SER:HB3	7	0.1
(2,210)	2:116:B:SER:H	2:111:B:ALA:HB1	9	0.1
(2,202)	2:114:B:GLY:H	2:115:B:ASN:HB3	8	0.1
(2,166)	1:43:A:TRP:HE1	1:39:A:VAL:HG13	10	0.1
(2,34)	1:12:A:SER:H	1:11:A:TYR:HD2	1	0.1
(1,93)	2:145:B:GLU:N	2:141:B:LYS:O	10	0.1
(1,82)	2:129:B:SER:H	2:125:B:LYS:O	4	0.1
(1,75)	2:126:B:ILE:N	2:122:B:ASP:O	8	0.1
(1,75)	2:126:B:ILE:N	2:122:B:ASP:O	9	0.1
(1,74)	2:125:B:LYS:H	2:121:B:LYS:O	3	0.1
(1,73)	2:125:B:LYS:N	2:121:B:LYS:O	7	0.1
(1,56)	2:107:B:TYR:H	2:103:B:TYR:O	8	0.1
(1,32)	1:31:A:LEU:H	1:27:A:LYS:O	7	0.1
(1,6)	1:9:A:CYS:H	1:5:A:SER:O	8	0.1

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

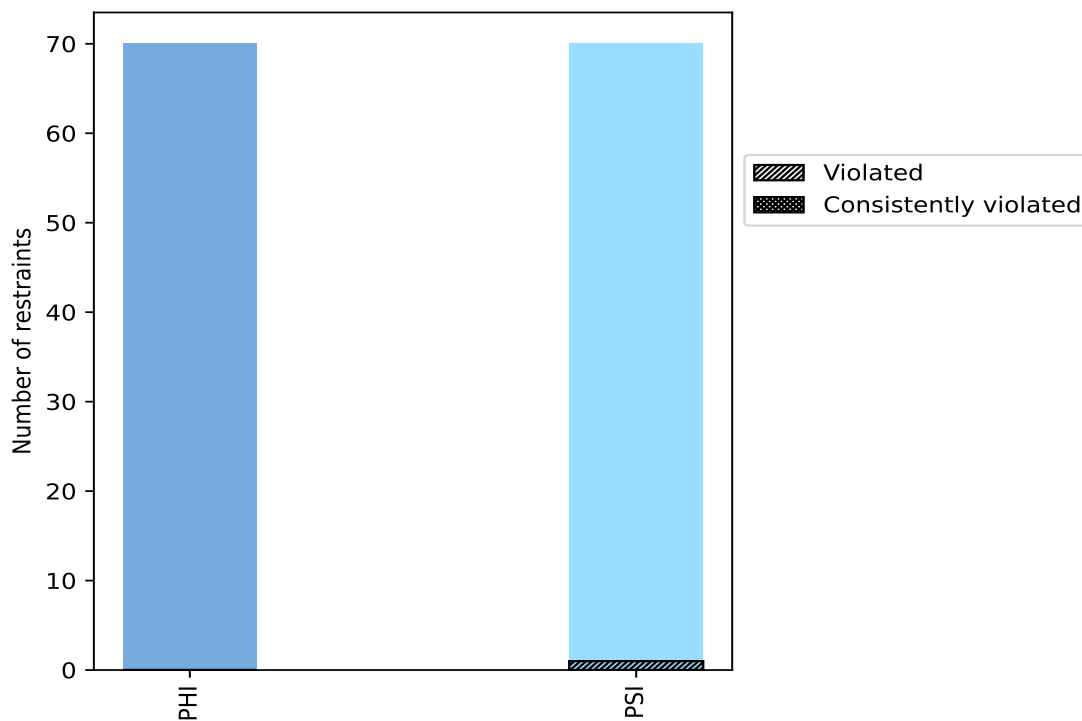
### 10.1 Summary of dihedral-angle violations [i](#)

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	70	50.0	0	0.0	0.0	0	0.0	0.0
PSI	70	50.0	1	1.4	0.7	0	0.0	0.0
Total	140	100.0	1	0.7	0.7	0	0.0	0.0

<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](#)



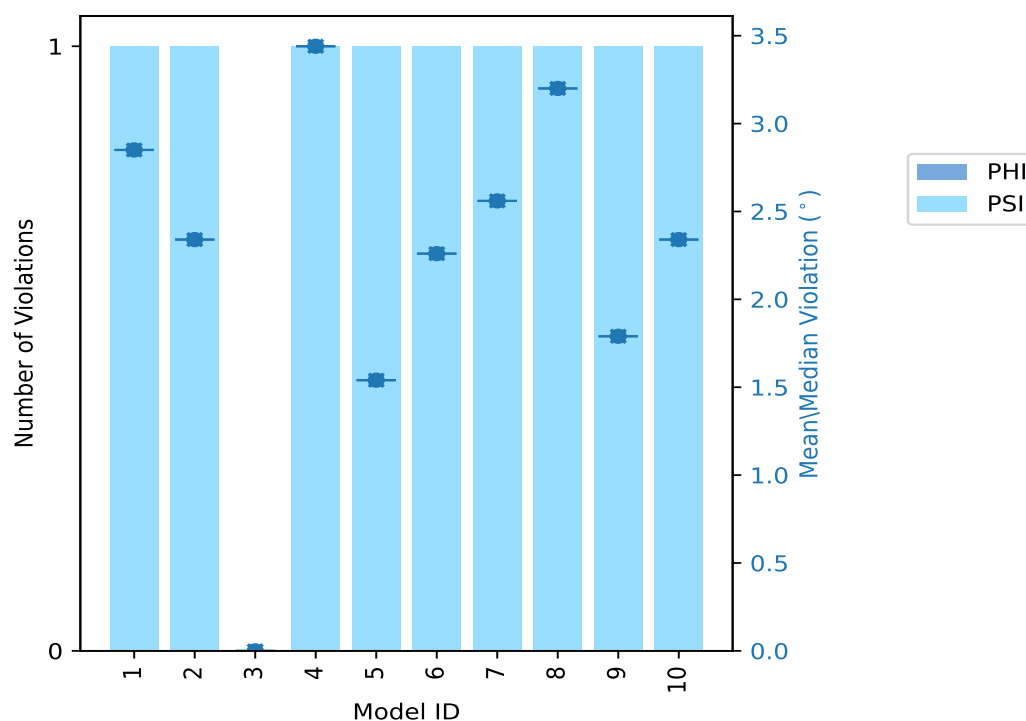
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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	0	1	1	2.85	2.85	0.0	2.85
2	0	1	1	2.34	2.34	0.0	2.34
3	0	0	0	0.0	0.0	0.0	0.0
4	0	1	1	3.44	3.44	0.0	3.44
5	0	1	1	1.54	1.54	0.0	1.54
6	0	1	1	2.26	2.26	0.0	2.26
7	0	1	1	2.56	2.56	0.0	2.56
8	0	1	1	3.2	3.2	0.0	3.2
9	0	1	1	1.79	1.79	0.0	1.79
10	0	1	1	2.34	2.34	0.0	2.34

### 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

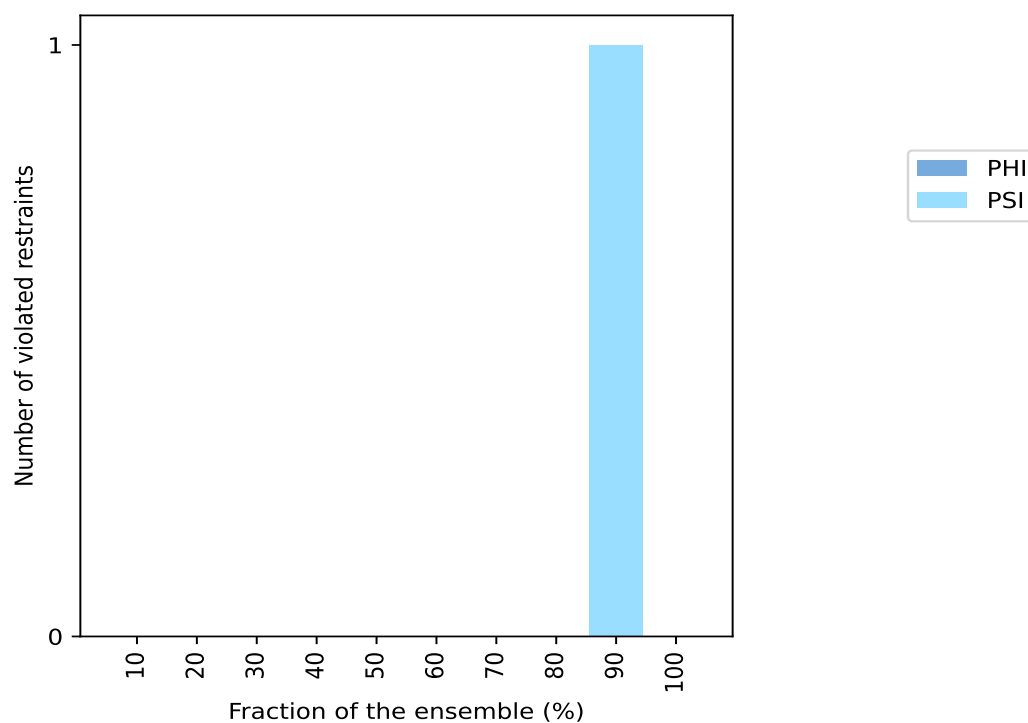
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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>	%
0	0	0	1	10.0
0	0	0	2	20.0
0	0	0	3	30.0
0	0	0	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
0	1	1	9	90.0
0	0	0	10	100.0

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

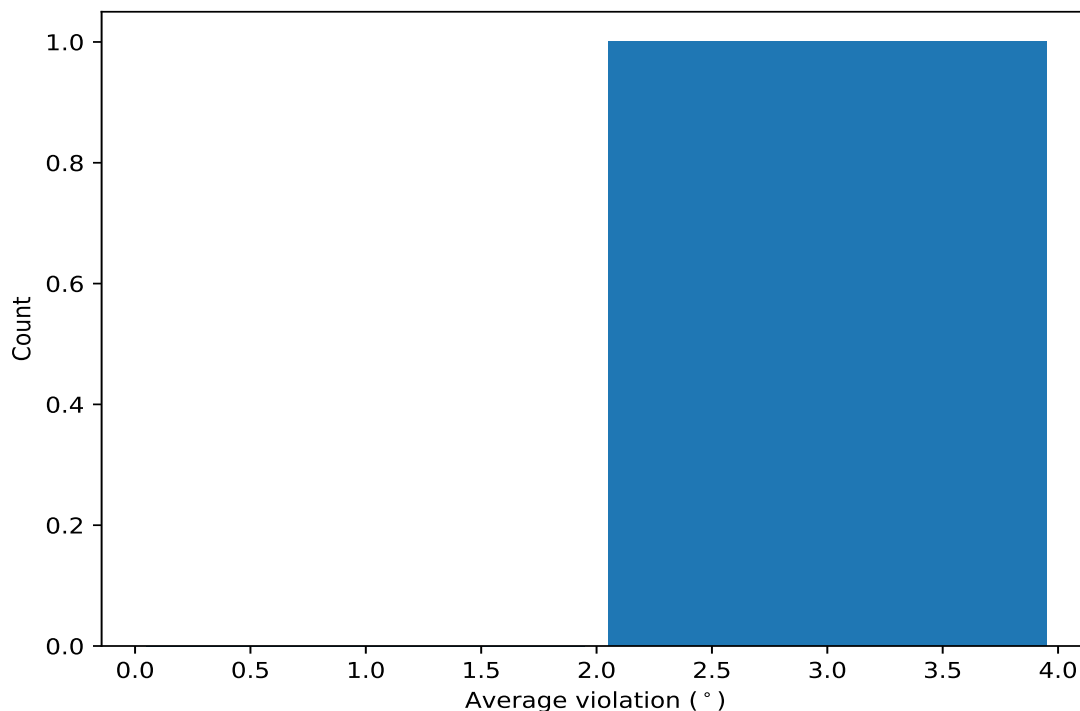
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

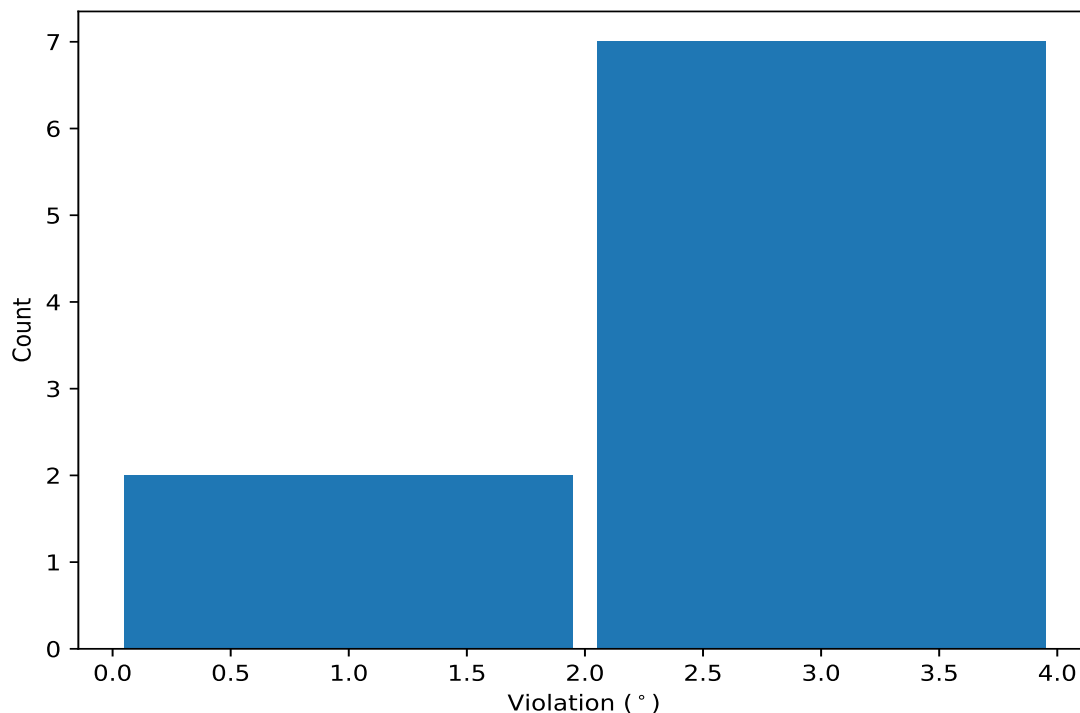
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	9	2.48	0.58	2.34

<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 [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	4	3.44
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	8	3.2
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	1	2.85
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	7	2.56
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	2	2.34
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	10	2.34
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	6	2.26
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	9	1.79
(1,138)	2:158:B:GLY:N	2:158:B:GLY:CA	2:158:B:GLY:C	2:159:B:ILE:N	5	1.54