



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 04:22 AM EST

PDB ID : 5MNW  
BMRB ID : 34077  
Title : Solution structure of the cinaciguat bound human beta1 H-NOX.  
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Deposited on : 2016-12-13

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

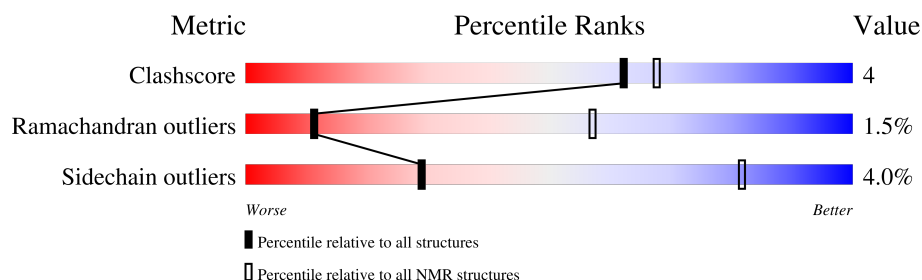
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 75%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	194	 94%

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:187 (187)	1.94	4

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



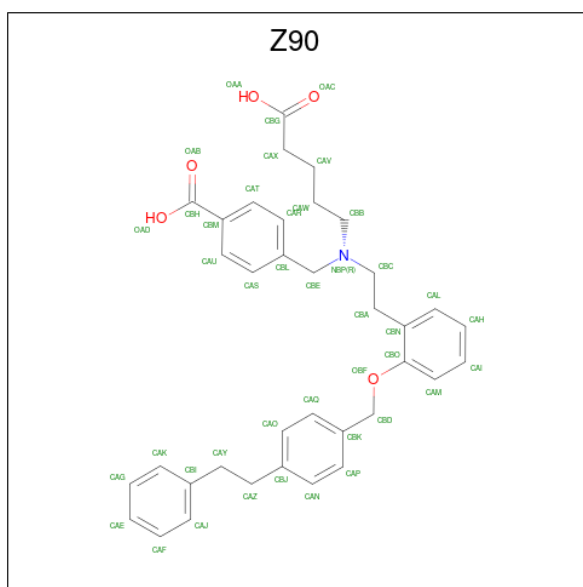
- Molecule 1 is a protein called Guanylate cyclase soluble subunit beta-1.

Mol	Chain	Residues	Atoms						Trace
1	A	194	Total	C	H	N	O	S	0
			3132	1003	1552	272	297	8	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	HIS	-	expression tag	UNP Q02153
A	190	HIS	-	expression tag	UNP Q02153
A	191	HIS	-	expression tag	UNP Q02153
A	192	HIS	-	expression tag	UNP Q02153
A	193	HIS	-	expression tag	UNP Q02153
A	194	HIS	-	expression tag	UNP Q02153

- Molecule 2 is 4-({(4-carboxybutyl)[2-(2-{[4-(2-phenylethyl)benzyl]oxy}phenyl)ethyl]amino}methyl)benzoic acid (three-letter code: Z90) (formula:  $\text{C}_{36}\text{H}_{39}\text{NO}_5$ ).



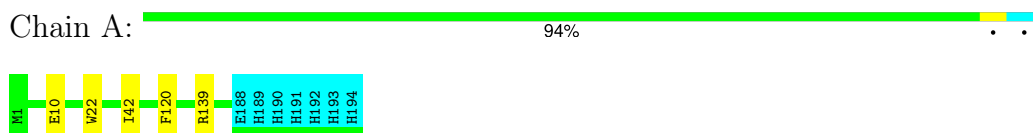
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			79	36	37	1	5

## 4 Residue-property plots

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

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

- Molecule 1: Guanylate cyclase soluble subunit beta-1

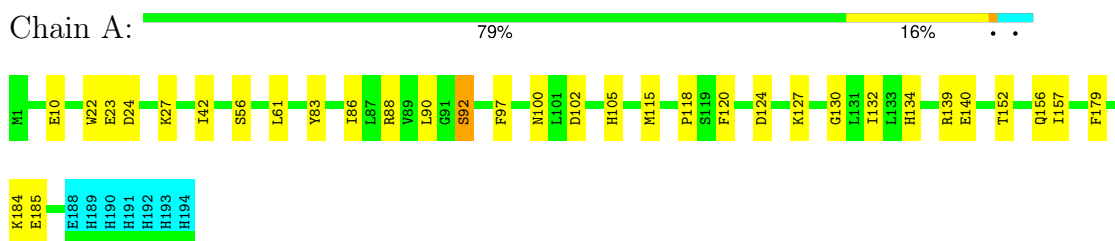


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

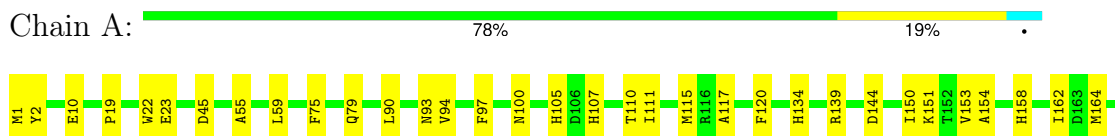
#### 4.2.1 Score per residue for model 1

- Molecule 1: Guanylate cyclase soluble subunit beta-1



#### 4.2.2 Score per residue for model 2

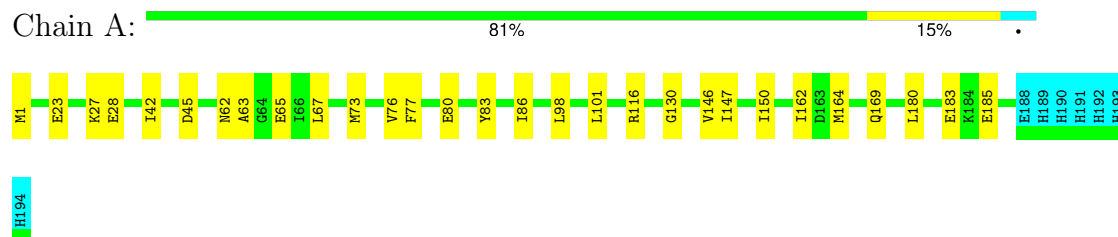
- Molecule 1: Guanylate cyclase soluble subunit beta-1





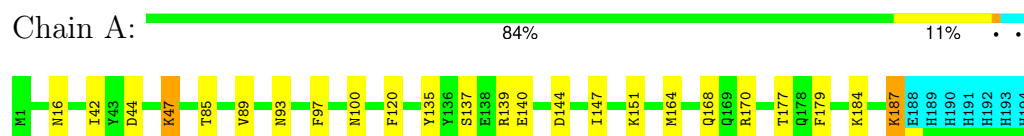
### 4.2.3 Score per residue for model 3

- Molecule 1: Guanylate cyclase soluble subunit beta-1



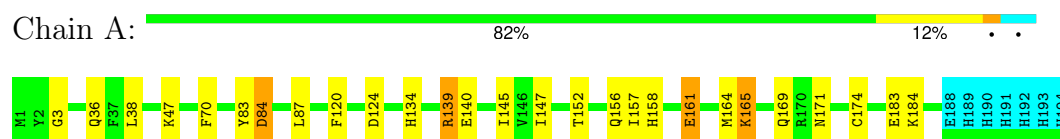
### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Guanylate cyclase soluble subunit beta-1



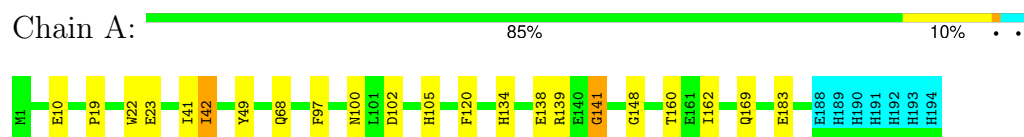
### 4.2.5 Score per residue for model 5

- Molecule 1: Guanylate cyclase soluble subunit beta-1



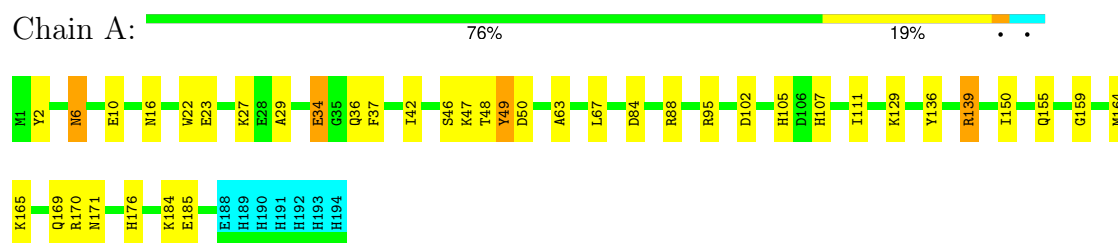
### 4.2.6 Score per residue for model 6

- Molecule 1: Guanylate cyclase soluble subunit beta-1



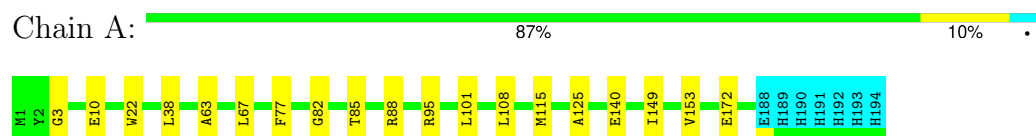
### 4.2.7 Score per residue for model 7

- Molecule 1: Guanylate cyclase soluble subunit beta-1



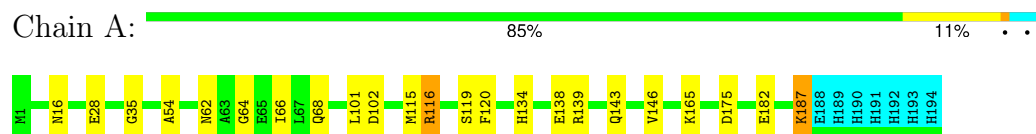
### 4.2.8 Score per residue for model 8

- Molecule 1: Guanylate cyclase soluble subunit beta-1



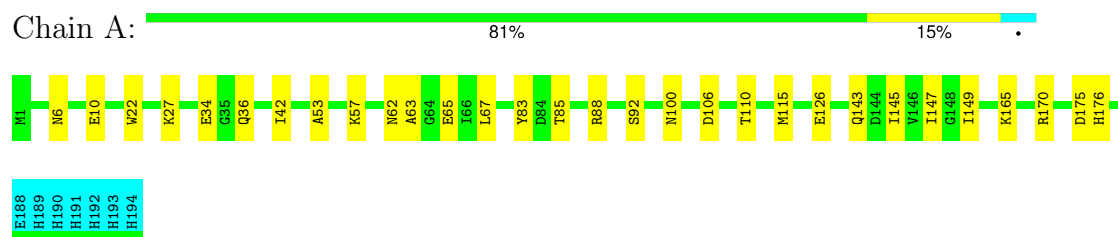
### 4.2.9 Score per residue for model 9

- Molecule 1: Guanylate cyclase soluble subunit beta-1



### 4.2.10 Score per residue for model 10

- Molecule 1: Guanylate cyclase soluble subunit beta-1



## 5 Refinement protocol and experimental data overview

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

Of the 200 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	structure calculation	1.21

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	3
Total number of shifts	2557
Number of shifts mapped to atoms	2557
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%



## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Z90

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	0.31±0.03	0±1/1538 ( 0.0± 0.0%)	0.38±0.01	0±0/2074 ( 0.0± 0.0%)
All	All	0.31	2/15380 ( 0.0%)	0.38	0/20740 ( 0.0%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	49	TYR	CE2-CZ	-6.57	1.30	1.38	7	1
1	A	49	TYR	CE1-CZ	5.82	1.46	1.38	7	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1510	1498	1492	11±3
2	A	42	37	37	2±1
All	All	15520	15350	15290	126

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ASP:OD1	1:A:119:SER:HB3	0.66	1.89	9	1
1:A:147:ILE:HA	1:A:164:MET:SD	0.64	2.31	5	2
1:A:84:ASP:O	1:A:87:LEU:HG	0.64	1.93	5	1
2:A:201:Z90:HAXA	2:A:201:Z90:NBP	0.63	2.09	1	2
1:A:150:ILE:HB	1:A:164:MET:SD	0.62	2.34	7	2
1:A:63:ALA:O	1:A:67:LEU:HG	0.61	1.95	3	3
1:A:120:PHE:HA	1:A:134:HIS:O	0.58	1.98	1	3
1:A:46:SER:HA	1:A:49:TYR:CD2	0.57	2.34	7	1
1:A:162:ILE:HG22	1:A:183:GLU:HA	0.57	1.77	6	2
1:A:23:GLU:O	1:A:27:LYS:HG2	0.56	2.00	1	2
1:A:23:GLU:O	1:A:27:LYS:HD3	0.56	2.01	3	1
1:A:137:SER:O	1:A:170:ARG:HD2	0.55	2.00	4	1
1:A:53:ALA:O	1:A:57:LYS:HG3	0.55	2.02	10	1
1:A:62:ASN:O	1:A:65:GLU:HG2	0.54	2.02	3	2
1:A:93:ASN:O	1:A:97:PHE:HB2	0.53	2.03	4	2
1:A:102:ASP:HA	1:A:105:HIS:ND1	0.53	2.19	6	1
1:A:152:THR:O	1:A:156:GLN:HB2	0.52	2.04	5	2
2:A:201:Z90:HBBA	2:A:201:Z90:CAR	0.51	2.34	4	2
1:A:83:TYR:O	1:A:86:ILE:HG12	0.51	2.04	3	1
1:A:164:MET:HA	1:A:180:LEU:O	0.51	2.06	3	1
1:A:10:GLU:HG2	1:A:22:TRP:CZ2	0.51	2.40	8	3
1:A:94:VAL:HG22	1:A:154:ALA:HA	0.51	1.82	2	1
1:A:73:MET:SD	1:A:77:PHE:HB2	0.50	2.47	3	1
1:A:56:SER:HA	1:A:61:LEU:O	0.49	2.06	1	1
1:A:146:VAL:O	1:A:150:ILE:HG12	0.49	2.06	3	1
1:A:68:GLN:NE2	1:A:148:GLY:HA2	0.49	2.22	6	1
1:A:106:ASP:HA	1:A:110:THR:O	0.49	2.07	10	1
1:A:47:LYS:NZ	1:A:47:LYS:HB2	0.49	2.23	5	1
2:A:201:Z90:CBG	2:A:201:Z90:CBB	0.49	2.91	4	2
1:A:102:ASP:O	1:A:105:HIS:HB3	0.49	2.08	1	2
1:A:3:GLY:HA3	1:A:38:LEU:O	0.49	2.08	5	2
1:A:149:ILE:O	1:A:153:VAL:HG13	0.48	2.08	8	1
1:A:75:PHE:CD1	1:A:153:VAL:HG12	0.48	2.44	2	1
1:A:90:LEU:HD13	1:A:97:PHE:CE2	0.48	2.44	2	2
1:A:143:GLN:O	1:A:147:ILE:HG12	0.48	2.08	10	1
2:A:201:Z90:NBP	2:A:201:Z90:CAX	0.47	2.77	10	2
1:A:161:GLU:O	1:A:184:LYS:HD3	0.47	2.08	5	1
1:A:85:THR:O	1:A:88:ARG:HG2	0.47	2.09	8	1
1:A:143:GLN:O	1:A:146:VAL:HG12	0.47	2.09	9	1
1:A:147:ILE:HD13	1:A:164:MET:SD	0.47	2.50	4	1
1:A:165:LYS:N	1:A:165:LYS:HD3	0.46	2.25	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LEU:O	1:A:101:LEU:HG	0.46	2.11	3	1
2:A:201:Z90:CAS	2:A:201:Z90:HAVA	0.46	2.40	5	1
1:A:107:HIS:O	1:A:111:ILE:HG13	0.46	2.10	2	2
1:A:187:LYS:HD3	1:A:187:LYS:H	0.46	1.69	9	1
2:A:201:Z90:CAS	2:A:201:Z90:CBC	0.46	2.94	9	1
1:A:41:ILE:O	1:A:42:ILE:HB	0.46	2.11	6	1
1:A:64:GLY:O	1:A:68:GLN:HG2	0.46	2.11	9	1
1:A:147:ILE:O	1:A:151:LYS:HG2	0.46	2.10	4	1
1:A:136:TYR:CE1	1:A:171:ASN:HA	0.45	2.45	7	1
2:A:201:Z90:CBG	2:A:201:Z90:HBB	0.45	2.40	2	1
1:A:85:THR:O	1:A:89:VAL:HG23	0.45	2.11	4	1
1:A:84:ASP:O	1:A:88:ARG:HB2	0.45	2.10	7	1
1:A:88:ARG:HA	1:A:88:ARG:NE	0.45	2.27	1	1
1:A:55:ALA:O	1:A:59:LEU:HB3	0.45	2.12	2	1
1:A:75:PHE:O	1:A:79:GLN:HG2	0.45	2.12	2	1
1:A:63:ALA:O	1:A:67:LEU:HD13	0.45	2.12	8	1
2:A:201:Z90:CAW	2:A:201:Z90:HBA	0.45	2.41	7	1
1:A:92:SER:O	1:A:157:ILE:HG21	0.44	2.12	1	1
1:A:120:PHE:HB2	1:A:134:HIS:O	0.44	2.13	9	2
1:A:1:MET:N	1:A:45:ASP:HA	0.44	2.27	3	1
1:A:135:TYR:O	1:A:177:THR:HB	0.44	2.11	4	1
1:A:19:PRO:O	1:A:23:GLU:HG3	0.44	2.11	2	1
1:A:49:TYR:OH	1:A:139:ARG:HA	0.44	2.11	7	1
1:A:170:ARG:HB2	1:A:176:HIS:O	0.44	2.13	2	3
1:A:49:TYR:CE1	1:A:141:GLY:HA3	0.44	2.48	6	1
1:A:115:MET:SD	1:A:116:ARG:N	0.43	2.91	9	1
1:A:171:ASN:HB3	1:A:174:CYS:SG	0.43	2.54	5	1
1:A:70:PHE:CD2	1:A:145:ILE:HD12	0.43	2.48	5	1
1:A:10:GLU:HG3	1:A:22:TRP:NE1	0.43	2.28	2	1
1:A:83:TYR:O	1:A:86:ILE:HG22	0.43	2.14	1	1
1:A:88:ARG:HA	1:A:92:SER:OG	0.43	2.13	10	1
1:A:147:ILE:HD11	1:A:179:PHE:CD2	0.43	2.49	4	1
2:A:201:Z90:CAR	2:A:201:Z90:CBB	0.42	2.96	4	1
1:A:160:THR:HG23	1:A:162:ILE:HG23	0.42	1.90	6	1
1:A:77:PHE:O	1:A:82:GLY:HA2	0.42	2.15	8	1
1:A:105:HIS:CD2	1:A:117:ALA:HB3	0.42	2.50	2	1
1:A:19:PRO:O	1:A:23:GLU:HG2	0.42	2.14	6	1
2:A:201:Z90:CAR	2:A:201:Z90:HAW	0.42	2.45	5	1
1:A:129:LYS:HD2	1:A:129:LYS:N	0.42	2.30	7	1
1:A:2:TYR:HE2	1:A:115:MET:SD	0.42	2.38	2	1
1:A:116:ARG:HB3	1:A:138:GLU:OE2	0.42	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:ILE:O	1:A:149:ILE:HG12	0.42	2.15	10	1
1:A:132:ILE:HA	1:A:179:PHE:O	0.41	2.14	1	1
1:A:94:VAL:CG2	1:A:154:ALA:HA	0.41	2.45	2	1
1:A:151:LYS:HE3	1:A:162:ILE:O	0.41	2.15	2	1
1:A:10:GLU:HG3	1:A:22:TRP:CE2	0.41	2.50	6	2
1:A:76:VAL:O	1:A:80:GLU:HG3	0.41	2.16	3	1
1:A:34:GLU:HG2	1:A:37:PHE:CZ	0.41	2.50	7	1
1:A:2:TYR:HA	1:A:6:ASN:HB2	0.41	1.92	7	1
1:A:62:ASN:O	1:A:66:ILE:HG13	0.41	2.16	9	1
1:A:2:TYR:OH	1:A:47:LYS:HB2	0.41	2.16	7	1
1:A:1:MET:HG3	1:A:45:ASP:OD1	0.41	2.15	2	1
1:A:108:LEU:HB3	1:A:115:MET:SD	0.41	2.56	8	1
2:A:201:Z90:HAVA	2:A:201:Z90:CBL	0.40	2.45	5	1
1:A:155:GLN:O	1:A:159:GLY:HA2	0.40	2.15	7	1
1:A:44:ASP:HB2	1:A:47:LYS:HD3	0.40	1.92	4	1
1:A:187:LYS:HD3	1:A:187:LYS:N	0.40	2.32	4	1
1:A:28:GLU:HB3	1:A:54:ALA:HB1	0.40	1.93	9	1
1:A:139:ARG:H	1:A:139:ARG:HD3	0.40	1.76	5	1
1:A:29:ALA:HA	1:A:50:ASP:OD2	0.40	2.16	7	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	186/194 (96%)	170±4 (91±2%)	14±5 (7±3%)	3±2 (1±1%)	11	57
All	All	1860/1940 (96%)	1697 (91%)	136 (7%)	27 (1%)	11	57

All 17 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	42	ILE	6
1	A	36	GLN	3
1	A	130	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	83	TYR	2
1	A	175	ASP	2
1	A	118	PRO	1
1	A	127	LYS	1
1	A	84	ASP	1
1	A	157	ILE	1
1	A	158	HIS	1
1	A	141	GLY	1
1	A	125	ALA	1
1	A	172	GLU	1
1	A	35	GLY	1
1	A	116	ARG	1
1	A	34	GLU	1
1	A	126	GLU	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	163/170 (96%)	156±2 (96±1%)	7±2 (4±1%)	29 82
All	All	1630/1700 (96%)	1564 (96%)	66 (4%)	29 82

All 33 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	139	ARG	7
1	A	100	ASN	5
1	A	169	GLN	5
1	A	140	GLU	4
1	A	165	LYS	4
1	A	184	LYS	3
1	A	185	GLU	3
1	A	16	ASN	3
1	A	115	MET	2
1	A	124	ASP	2
1	A	144	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	187	LYS	2
1	A	6	ASN	2
1	A	95	ARG	2
1	A	101	LEU	2
1	A	24	ASP	1
1	A	92	SER	1
1	A	110	THR	1
1	A	158	HIS	1
1	A	28	GLU	1
1	A	116	ARG	1
1	A	47	LYS	1
1	A	120	PHE	1
1	A	168	GLN	1
1	A	161	GLU	1
1	A	183	GLU	1
1	A	97	PHE	1
1	A	138	GLU	1
1	A	34	GLU	1
1	A	48	THR	1
1	A	182	GLU	1
1	A	27	LYS	1
1	A	85	THR	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds

that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	Z90	A	201	-	45,45,45	2.00±0.03	6±0 (13±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	Z90	A	201	-	58,58,58	0.95±0.04	2±0 (2±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Z90	A	201	-	-	0±0,30,30,30	0±0,4,4,4

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	Z90	CBE-CBL	6.72	1.39	1.51	6	10
2	A	201	Z90	CBA-CBN	6.65	1.39	1.51	6	10
2	A	201	Z90	CBM-CBH	4.93	1.39	1.49	9	10
2	A	201	Z90	CBD-CBK	4.88	1.39	1.50	1	10
2	A	201	Z90	CAZ-CBJ	4.47	1.39	1.51	8	10
2	A	201	Z90	CAY-CBI	4.44	1.39	1.51	8	10

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

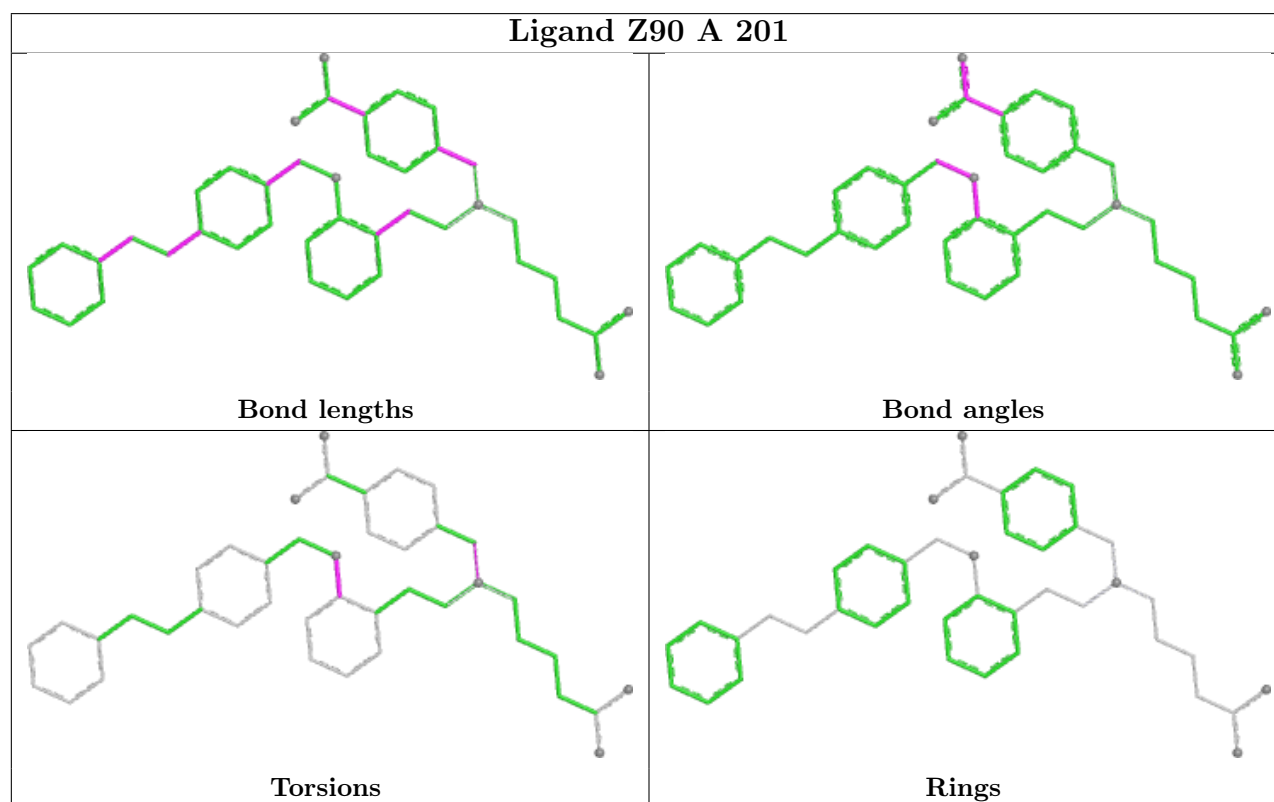
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	201	Z90	CBD-OBF-CBO	4.30	109.25	117.76	5	10
2	A	201	Z90	OAD-CBH-CBM	2.18	120.43	114.84	10	7

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 72% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *H-NOX\_A37C\_chemShift\_edited*

#### 7.1.1 Bookkeeping

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

Total number of shifts	560
Number of shifts mapped to atoms	560
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	163	$-0.64 \pm 0.06$	Should be checked
$^{13}\text{C}_\beta$	1	—	None (insufficient data)
$^{13}\text{C}'$	2	—	None (insufficient data)
$^{15}\text{N}$	163	$0.52 \pm 0.27$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 21%, i.e. 558 atoms were assigned a chemical shift out of a possible 2624. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	494/942 (52%)	167/384 (43%)	165/374 (44%)	162/184 (88%)
Sidechain	62/1460 (4%)	41/947 (4%)	8/460 (2%)	13/53 (25%)

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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	2/222 (1%)	1/107 (1%)	0/102 (0%)	1/13 (8%)
Overall	558/2624 (21%)	209/1438 (15%)	173/936 (18%)	176/250 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 560 atoms were assigned a chemical shift out of a possible 2732. 0 out of 31 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	496/977 (51%)	168/398 (42%)	165/388 (43%)	163/191 (85%)
Sidechain	62/1485 (4%)	41/963 (4%)	8/469 (2%)	13/53 (25%)
Aromatic	2/270 (1%)	1/131 (1%)	0/114 (0%)	1/25 (4%)
Overall	560/2732 (20%)	210/1492 (14%)	173/971 (18%)	177/269 (66%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

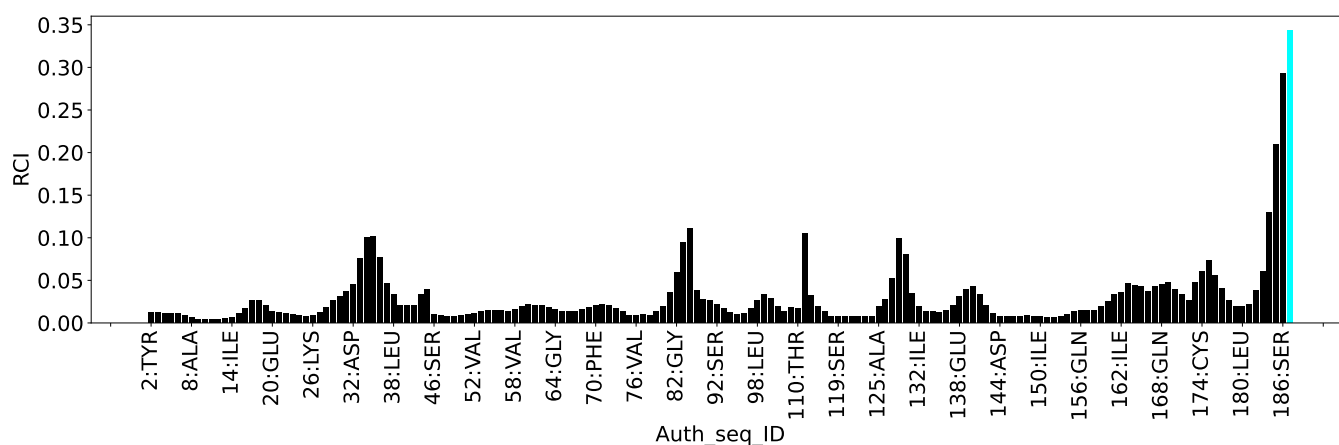
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	10	GLU	HA	1.72	2.24 – 6.23	-6.3

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

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

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *H-NOX\_B\_chemShift\_edited*

### 7.2.1 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	20
Number of shifts mapped to atoms	20
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2624. 0 out of 31 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	0/942 (0%)	0/384 (0%)	0/374 (0%)	0/184 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Sidechain	0/1460 (0%)	0/947 (0%)	0/460 (0%)	0/53 (0%)
Aromatic	0/222 (0%)	0/107 (0%)	0/102 (0%)	0/13 (0%)
Overall	0/2624 (0%)	0/1438 (0%)	0/936 (0%)	0/250 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2732. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/977 (0%)	0/398 (0%)	0/388 (0%)	0/191 (0%)
Sidechain	0/1485 (0%)	0/963 (0%)	0/469 (0%)	0/53 (0%)
Aromatic	0/270 (0%)	0/131 (0%)	0/114 (0%)	0/25 (0%)
Overall	0/2732 (0%)	0/1492 (0%)	0/971 (0%)	0/269 (0%)

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

There are no statistically unusual chemical shifts.

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

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

### 7.3 Chemical shift list 3

File name: working\_cs.cif

Chemical shift list name: *H-NOX\_A\_chemShift\_edited*

#### 7.3.1 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	1977
Number of shifts mapped to atoms	1977
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	177	$-0.33 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	160	$0.16 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	169	$-0.00 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	172	$0.24 \pm 0.37$	None needed ( $< 0.5$ ppm)

### 7.3.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 1965 atoms were assigned a chemical shift out of a possible 2624. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	868/942 (92%)	355/384 (92%)	343/374 (92%)	170/184 (92%)
Sidechain	1011/1460 (69%)	652/947 (69%)	344/460 (75%)	15/53 (28%)
Aromatic	86/222 (39%)	59/107 (55%)	26/102 (25%)	1/13 (8%)
Overall	1965/2624 (75%)	1066/1438 (74%)	713/936 (76%)	186/250 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1974 atoms were assigned a chemical shift out of a possible 2732. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	876/977 (90%)	358/398 (90%)	346/388 (89%)	172/191 (90%)
Sidechain	1012/1485 (68%)	652/963 (68%)	345/469 (74%)	15/53 (28%)
Aromatic	86/270 (32%)	59/131 (45%)	26/114 (23%)	1/25 (4%)
Overall	1974/2732 (72%)	1069/1492 (72%)	717/971 (74%)	188/269 (70%)

### 7.3.4 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
3	A	152	THR	HG1	5.74	0.08 – 2.19	21.8
3	A	48	THR	HG1	5.67	0.08 – 2.19	21.5
3	A	40	ARG	HG2	3.41	0.26 – 2.87	7.1

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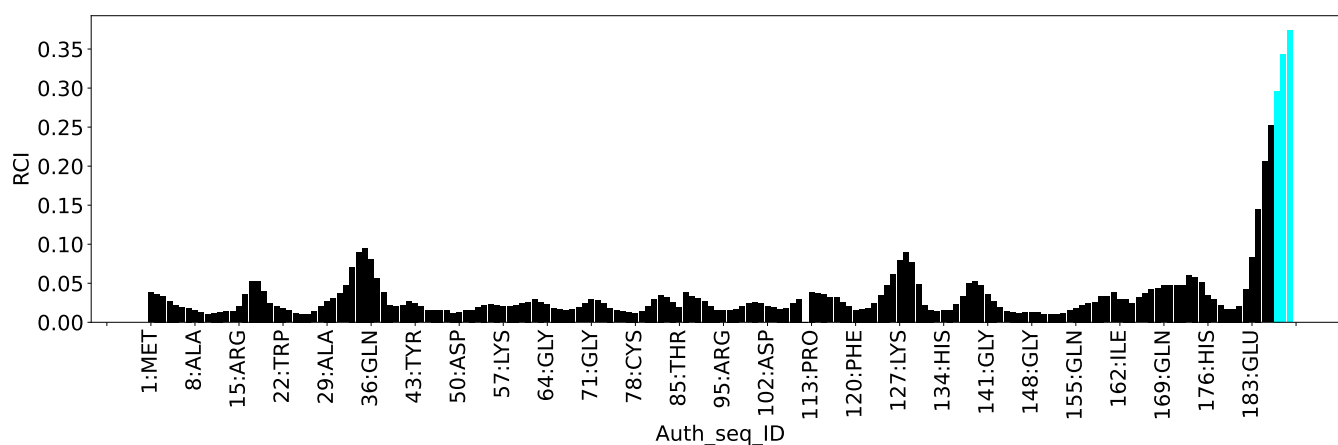
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
3	A	10	GLU	HG3	0.81	1.20 – 3.30	-6.9
3	A	10	GLU	HA	1.55	2.24 – 6.23	-6.8
3	A	40	ARG	HG3	3.42	0.15 – 2.94	6.7

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3600
Intra-residue ( $ i-j =0$ )	1180
Sequential ( $ i-j =1$ )	975
Medium range ( $ i-j >1$ and $ i-j <5$ )	665
Long range ( $ i-j \geq 5$ )	679
Inter-chain	96
Hydrogen bond restraints	5
Disulfide bond restraints	0
Total dihedral-angle restraints	265
Number of unmapped restraints	0
Number of restraints per residue	19.8
Number of long range restraints per residue <sup>1</sup>	3.5

<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)	77.0	0.2
0.2-0.5 (Medium)	160.4	0.5
>0.5 (Large)	259.4	12.06



### 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)	10.4	9.32
10.0-20.0 (Medium)	0.3	11.19
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

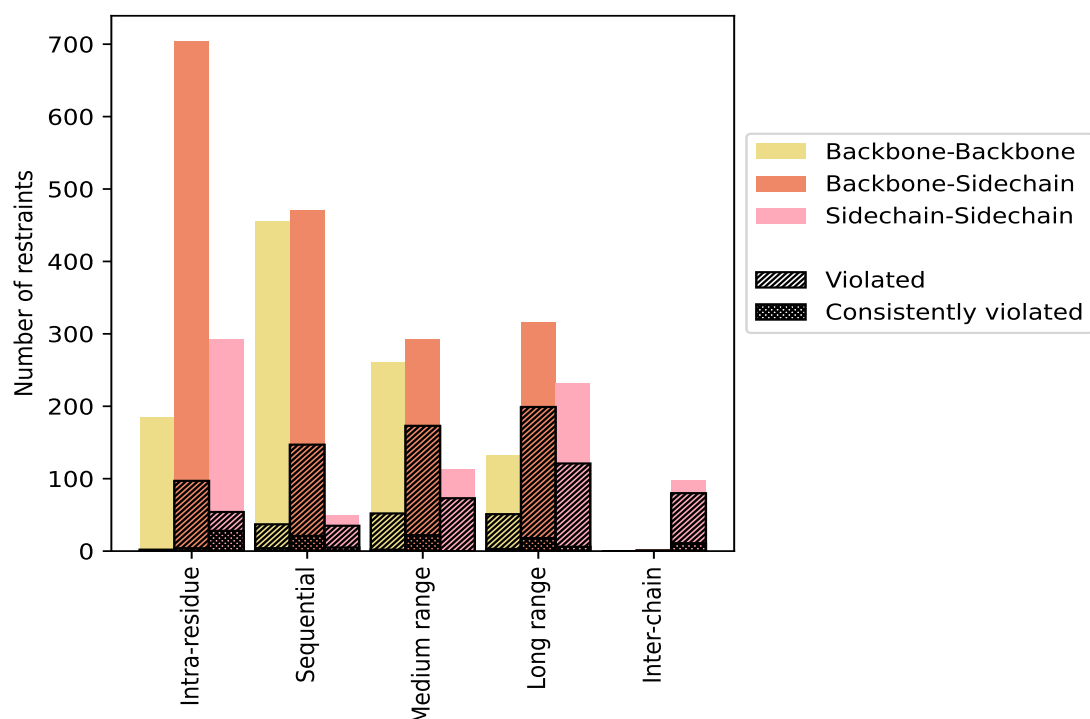
### 9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>1180</b>	<b>32.8</b>	<b>153</b>	<b>13.0</b>	<b>4.2</b>	<b>32</b>	<b>2.7</b>	<b>0.9</b>
Backbone-Backbone	184	5.1	2	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	704	19.6	97	13.8	2.7	4	0.6	0.1
Sidechain-Sidechain	292	8.1	54	18.5	1.5	28	9.6	0.8
<b>Sequential (<math> i-j =1</math>)</b>	<b>975</b>	<b>27.1</b>	<b>219</b>	<b>22.5</b>	<b>6.1</b>	<b>30</b>	<b>3.1</b>	<b>0.8</b>
Backbone-Backbone	455	12.6	37	8.1	1.0	4	0.9	0.1
Backbone-Sidechain	471	13.1	147	31.2	4.1	21	4.5	0.6
Sidechain-Sidechain	49	1.4	35	71.4	1.0	5	10.2	0.1
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>665</b>	<b>18.5</b>	<b>298</b>	<b>44.8</b>	<b>8.3</b>	<b>24</b>	<b>3.6</b>	<b>0.7</b>
Backbone-Backbone	260	7.2	52	20.0	1.4	2	0.8	0.1
Backbone-Sidechain	292	8.1	173	59.2	4.8	22	7.5	0.6
Sidechain-Sidechain	113	3.1	73	64.6	2.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>679</b>	<b>18.9</b>	<b>371</b>	<b>54.6</b>	<b>10.3</b>	<b>27</b>	<b>4.0</b>	<b>0.8</b>
Backbone-Backbone	132	3.7	51	38.6	1.4	3	2.3	0.1
Backbone-Sidechain	316	8.8	199	63.0	5.5	18	5.7	0.5
Sidechain-Sidechain	231	6.4	121	52.4	3.4	6	2.6	0.2
<b>Inter-chain</b>	<b>96</b>	<b>2.7</b>	<b>77</b>	<b>80.2</b>	<b>2.1</b>	<b>11</b>	<b>11.5</b>	<b>0.3</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.1	1	50.0	0.0	0	0.0	0.0
Sidechain-Sidechain	94	2.6	76	80.9	2.1	11	11.7	0.3
<b>Hydrogen bond</b>	<b>5</b>	<b>0.1</b>	<b>4</b>	<b>80.0</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</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>3600</b>	<b>100.0</b>	<b>1122</b>	<b>31.2</b>	<b>31.2</b>	<b>124</b>	<b>3.4</b>	<b>3.4</b>
Backbone-Backbone	1031	28.6	142	13.8	3.9	9	0.9	0.2
Backbone-Sidechain	1786	49.6	617	34.5	17.1	65	3.6	1.8
Sidechain-Sidechain	783	21.8	363	46.4	10.1	50	6.4	1.4

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

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



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

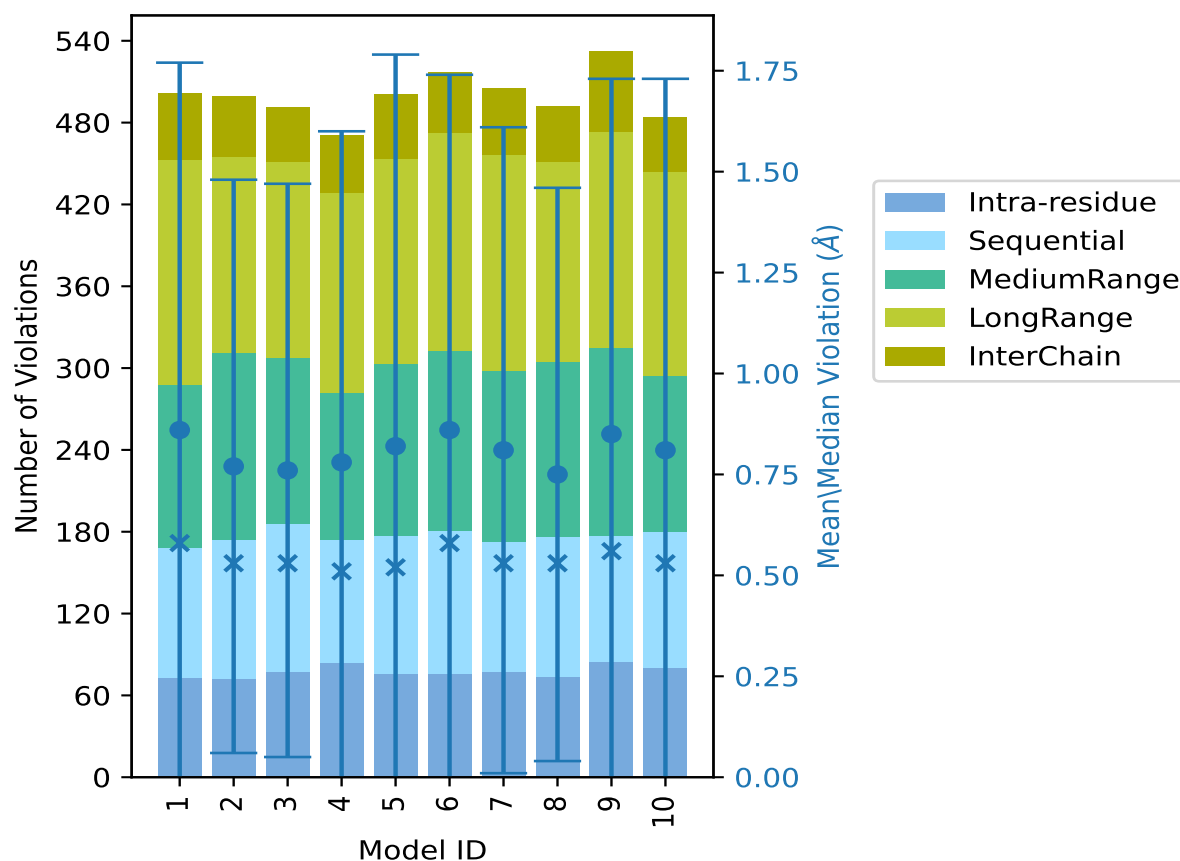
## 9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	73	95	120	165	49	502	0.86	8.59	0.91	0.58
2	72	102	137	144	44	499	0.77	4.53	0.71	0.53
3	77	109	122	143	40	491	0.76	4.41	0.71	0.53
4	84	90	108	147	42	471	0.78	5.6	0.82	0.51
5	76	101	126	151	47	501	0.82	12.06	0.97	0.52
6	76	105	132	160	44	517	0.86	5.93	0.88	0.58
7	77	96	125	158	49	505	0.81	5.35	0.8	0.53
8	74	102	129	146	41	492	0.75	6.62	0.71	0.53
9	85	92	138	158	59	532	0.85	6.26	0.88	0.56
10	80	100	114	150	40	484	0.81	11.71	0.92	0.53

<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, 2477(IR:1027, SQ:756, MR:367, LR:308, IC:19) 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>	%
32	51	73	88	7	251	1	10.0
21	29	44	71	8	173	2	20.0
17	29	39	37	7	129	3	30.0

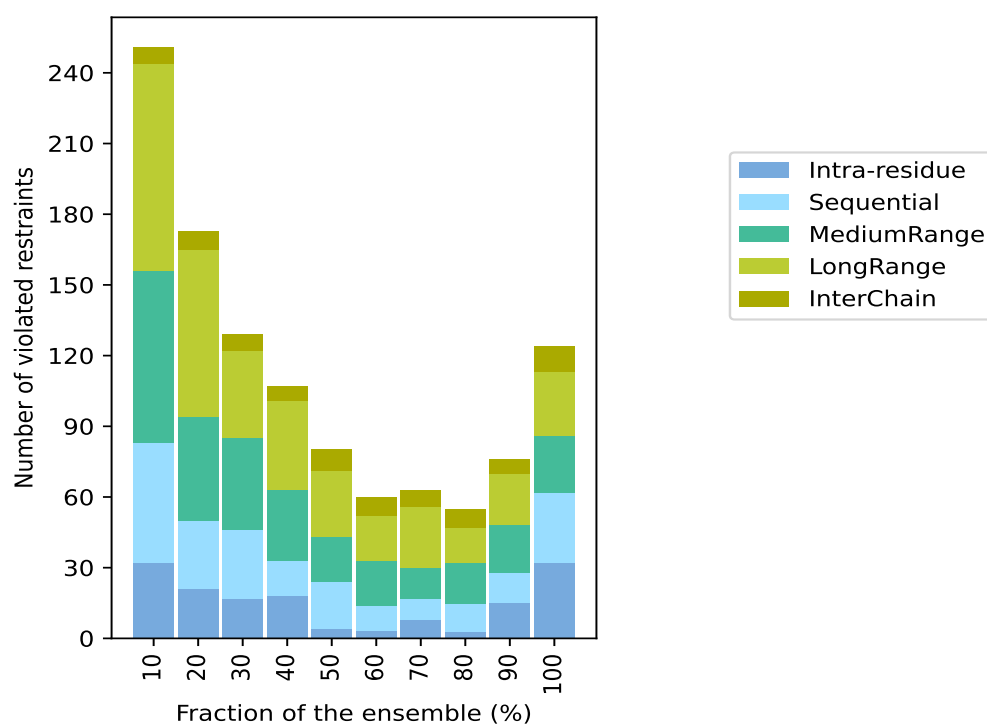
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
18	15	30	38	6	107	4	40.0
4	20	19	28	9	80	5	50.0
3	11	19	19	8	60	6	60.0
8	9	13	26	7	63	7	70.0
3	12	17	15	8	55	8	80.0
15	13	20	22	6	76	9	90.0
32	30	24	27	11	124	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](#)

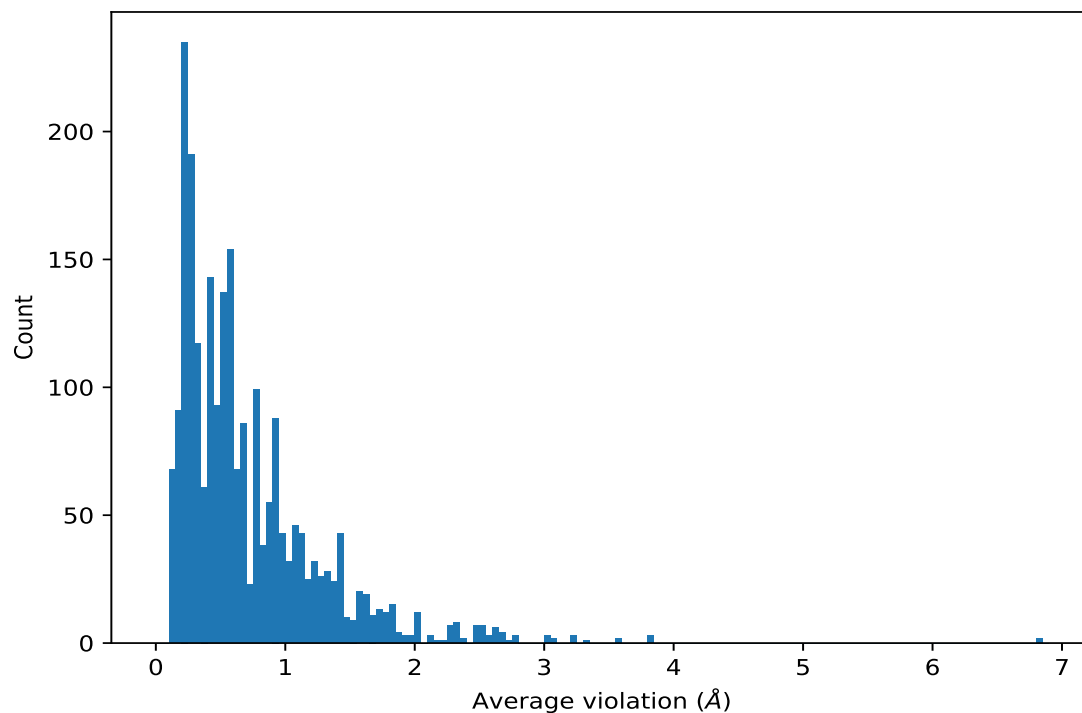


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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)
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	10	6.82	2.83	5.6
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	10	6.82	2.83	5.6
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	10	3.01	0.57	3.03
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	10	3.01	0.57	3.03
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	10	3.01	0.57	3.03
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	10	2.68	0.91	2.72
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	10	2.68	0.91	2.72
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	10	2.68	0.91	2.72
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	10	2.64	0.66	2.76
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	10	2.62	1.48	2.3
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	10	2.62	1.48	2.3
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	10	2.6	0.78	2.87
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	10	2.6	0.78	2.87
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	10	2.6	0.78	2.87
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	10	2.59	0.57	2.61

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	10	2.59	0.57	2.61
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	10	2.59	0.57	2.61
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	10	2.55	1.65	2.46
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	10	2.55	1.65	2.46
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	10	2.55	1.65	2.46
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	10	2.55	1.47	2.51
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	10	2.55	1.47	2.51
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	10	2.55	1.47	2.51
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	10	2.53	0.49	2.38
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	10	2.46	0.82	2.46
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	10	2.46	0.82	2.46
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	10	2.45	0.5	2.3
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	10	2.25	0.49	2.33
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	10	2.25	0.49	2.33
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	10	2.25	0.49	2.33
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	10	2.04	0.5	2.04
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	10	2.04	0.5	2.04
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	10	2.04	0.5	2.04
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	10	2.03	0.66	2.14
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	10	2.03	0.66	2.14
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	10	1.84	0.87	1.68
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	10	1.84	0.87	1.68
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	10	1.84	0.87	1.68
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	10	1.79	0.82	1.78
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	10	1.74	0.42	1.66
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	10	1.74	0.42	1.66
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	10	1.74	0.42	1.66
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	10	1.65	0.79	2.26
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	10	1.65	0.79	2.26
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	10	1.65	0.79	2.26
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	10	1.62	0.5	1.7
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	10	1.58	0.64	1.52
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	10	1.55	0.54	1.61
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	10	1.55	0.54	1.61
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	10	1.55	0.54	1.61

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	10	1.53	0.51	1.77
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	10	1.45	0.66	1.27
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	10	1.45	0.66	1.27
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	10	1.43	0.77	1.22
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	10	1.43	0.77	1.22
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	10	1.43	0.77	1.22
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	10	1.43	0.77	1.22
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	10	1.43	0.77	1.22
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	10	1.43	0.77	1.22
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	10	1.41	0.52	1.48
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	10	1.41	0.52	1.48
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	10	1.41	0.52	1.48
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	10	1.37	0.77	1.13
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	10	1.37	0.77	1.13
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	10	1.34	0.76	1.6
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	10	1.33	0.3	1.25
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	10	1.33	0.27	1.32
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	10	1.3	0.14	1.27
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	10	1.29	0.13	1.27
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	10	1.26	0.07	1.27
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	10	1.26	0.07	1.27
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	10	1.26	0.07	1.27
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	10	1.23	0.55	1.06
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	10	1.22	0.13	1.2
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	10	1.2	0.32	1.06
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	10	1.18	0.56	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	10	1.18	0.56	1.2
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	10	1.17	0.5	1.06
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	10	1.17	0.5	1.06
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	10	1.17	0.5	1.06
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	10	1.16	0.43	1.23
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	10	1.16	0.43	1.23
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	10	1.16	0.43	1.23
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	10	1.13	0.58	1.18
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	10	1.13	0.33	1.07

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	10	1.12	0.8	0.88
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	10	1.11	0.41	1.09
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	10	1.11	0.41	1.09
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	10	1.11	0.41	1.09
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	10	1.06	0.17	1.08
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	10	1.04	0.39	1.12
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	10	1.03	0.23	0.99
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	10	1.03	0.48	1.0
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	10	1.03	0.47	0.93
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	10	1.0	0.23	0.96
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	10	1.0	0.41	1.04
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	10	1.0	0.41	1.04
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	10	1.0	0.41	1.04
(1,245)	1:69:A:MET:HE1	1:68:A:GLN:H	10	0.99	0.12	0.98
(1,245)	1:69:A:MET:HE2	1:68:A:GLN:H	10	0.99	0.12	0.98
(1,245)	1:69:A:MET:HE3	1:68:A:GLN:H	10	0.99	0.12	0.98
(1,245)	1:66:A:ILE:HB	1:68:A:GLN:H	10	0.99	0.12	0.98
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD21	10	0.97	0.22	0.96
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD22	10	0.97	0.22	0.96
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD23	10	0.97	0.22	0.96
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	10	0.97	0.22	0.96
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	10	0.97	0.22	0.96
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	10	0.97	0.22	0.96
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	10	0.96	0.41	1.0
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	10	0.96	0.41	1.0
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	10	0.96	0.41	1.0
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	10	0.95	0.28	0.96
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	10	0.94	0.19	0.93
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	10	0.94	0.19	0.93
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	10	0.94	0.19	0.93
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	10	0.92	0.08	0.91
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	10	0.9	0.48	0.87
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	10	0.9	0.36	0.83
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	10	0.87	0.41	0.82
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	10	0.87	0.32	0.86
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	10	0.87	0.32	0.86
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	10	0.87	0.32	0.86
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	10	0.83	0.14	0.82
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	10	0.83	0.22	0.84
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	10	0.83	0.22	0.84
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	10	0.83	0.22	0.84
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	10	0.83	0.15	0.8

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	10	0.8	0.35	0.74
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	10	0.8	0.11	0.78
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	10	0.78	0.36	0.74
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	10	0.78	0.24	0.7
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	10	0.78	0.24	0.7
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	10	0.78	0.24	0.7
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	10	0.77	0.22	0.72
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	10	0.77	0.22	0.72
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	10	0.77	0.22	0.72
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	10	0.73	0.19	0.68
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	10	0.72	0.08	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	10	0.72	0.08	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	10	0.72	0.08	0.72
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	10	0.7	0.1	0.72
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	10	0.69	0.33	0.63
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	10	0.69	0.33	0.63
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	10	0.67	0.15	0.71
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	10	0.67	0.15	0.71
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	10	0.67	0.15	0.71
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	10	0.65	0.21	0.64
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	10	0.65	0.21	0.64
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	10	0.65	0.21	0.64
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	10	0.64	0.18	0.64
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	10	0.64	0.18	0.64
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	10	0.64	0.18	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	10	0.64	0.05	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	10	0.64	0.05	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	10	0.64	0.05	0.64
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	10	0.64	0.23	0.63
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	10	0.63	0.02	0.62
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	10	0.63	0.02	0.62
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	10	0.61	0.24	0.62
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	10	0.61	0.17	0.64
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	10	0.61	0.17	0.64
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	10	0.61	0.17	0.64
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	10	0.61	0.05	0.6
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	10	0.61	0.05	0.6
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	10	0.61	0.05	0.6
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	10	0.6	0.0	0.6
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	10	0.59	0.22	0.61
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	10	0.59	0.22	0.61
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	10	0.59	0.22	0.61

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	10	0.58	0.07	0.57
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	10	0.58	0.07	0.57
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	10	0.58	0.07	0.57
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	10	0.58	0.17	0.62
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	10	0.58	0.17	0.62
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	10	0.58	0.17	0.62
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	10	0.54	0.02	0.54
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	10	0.54	0.02	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	10	0.53	0.01	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	10	0.53	0.01	0.54
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	10	0.53	0.01	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	10	0.53	0.01	0.53
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	10	0.52	0.07	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	10	0.52	0.07	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	10	0.52	0.07	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	10	0.52	0.07	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	10	0.52	0.07	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	10	0.52	0.07	0.57
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	10	0.5	0.0	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	10	0.5	0.0	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	10	0.5	0.0	0.5
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	10	0.49	0.07	0.48
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	10	0.49	0.07	0.48
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	10	0.49	0.07	0.48
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	10	0.49	0.07	0.48
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	10	0.49	0.07	0.48
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	10	0.49	0.07	0.48
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	10	0.49	0.08	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	10	0.49	0.08	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	10	0.49	0.08	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	10	0.49	0.09	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	10	0.49	0.09	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	10	0.49	0.09	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	10	0.49	0.09	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	10	0.49	0.09	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	10	0.49	0.09	0.49
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	10	0.48	0.0	0.48
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	10	0.46	0.28	0.36
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	10	0.46	0.28	0.36
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	10	0.46	0.28	0.36
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	10	0.44	0.22	0.42
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	10	0.44	0.22	0.42

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	10	0.43	0.19	0.44
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	10	0.42	0.0	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	10	0.42	0.0	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	10	0.42	0.0	0.42
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	10	0.41	0.03	0.41
(1,121)	1:30:A:GLN:HG2	1:31:A:LEU:H	10	0.41	0.03	0.41
(1,121)	1:30:A:GLN:HG3	1:31:A:LEU:H	10	0.41	0.03	0.41
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	10	0.4	0.0	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	10	0.4	0.0	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	10	0.4	0.0	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	10	0.4	0.0	0.4
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	10	0.39	0.0	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	10	0.39	0.0	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	10	0.39	0.0	0.39
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	10	0.38	0.03	0.38
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	10	0.38	0.03	0.38
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	10	0.36	0.01	0.36
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	10	0.36	0.02	0.36
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	10	0.35	0.14	0.32
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	10	0.35	0.0	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	10	0.35	0.0	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	10	0.35	0.0	0.35
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	10	0.32	0.08	0.31
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	10	0.32	0.08	0.31
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	10	0.31	0.05	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	10	0.3	0.0	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	10	0.3	0.0	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	10	0.3	0.0	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	10	0.3	0.0	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	10	0.3	0.0	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	10	0.3	0.0	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	10	0.3	0.0	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	10	0.3	0.0	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	10	0.3	0.0	0.3
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	10	0.3	0.11	0.34
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	10	0.29	0.0	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	10	0.29	0.0	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	10	0.29	0.0	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	10	0.29	0.0	0.29
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	10	0.25	0.06	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	10	0.25	0.06	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	10	0.25	0.06	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	10	0.22	0.01	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	10	0.22	0.01	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	10	0.22	0.01	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	10	0.22	0.01	0.22
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	10	0.22	0.04	0.23
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	10	0.21	0.0	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	10	0.21	0.0	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	10	0.21	0.0	0.21
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	10	0.2	0.05	0.22
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	10	0.19	0.01	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	10	0.19	0.01	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	10	0.19	0.01	0.2
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	10	0.18	0.0	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	10	0.18	0.0	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	10	0.18	0.0	0.18
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	10	0.14	0.0	0.14
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	10	0.13	0.0	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	10	0.13	0.0	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	10	0.13	0.0	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	10	0.13	0.0	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	10	0.13	0.0	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	10	0.13	0.0	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	10	0.13	0.01	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	10	0.13	0.01	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	10	0.13	0.01	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	10	0.13	0.01	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	10	0.13	0.01	0.13
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	9	3.84	1.1	4.09
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	9	3.84	1.1	4.09
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	9	3.84	1.1	4.09
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	9	3.58	1.49	3.28
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	9	3.58	1.49	3.28
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	9	3.2	1.6	2.67
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	9	3.2	1.6	2.67
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	9	3.2	1.6	2.67
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	9	2.47	1.74	3.32
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	9	2.47	1.74	3.32
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	9	2.47	1.74	3.32
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	9	2.33	1.48	2.2
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	9	2.33	1.48	2.2
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	9	2.17	0.93	1.87
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	9	1.83	0.85	2.07

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	9	1.83	0.85	2.07
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	9	1.83	0.85	2.07
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	9	1.83	0.85	2.07
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	9	1.83	0.85	2.07
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	9	1.83	0.85	2.07
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	9	1.81	0.14	1.83
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	9	1.67	0.35	1.74
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	9	1.67	0.35	1.74
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	9	1.61	0.97	1.53
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	9	1.61	0.97	1.53
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	9	1.61	0.97	1.53
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	9	1.5	0.84	0.99
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD1	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD2	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD1	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD2	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD1	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD2	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:H	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:H	9	1.39	0.46	1.31
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:H	9	1.39	0.46	1.31
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	9	1.34	0.35	1.35
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	9	1.34	0.35	1.35
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	9	1.34	0.35	1.35
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	9	1.32	0.39	1.23
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	9	1.28	0.65	1.12
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	9	1.28	0.65	1.12
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	9	1.28	0.65	1.12
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	9	1.27	0.3	1.24
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	9	1.25	0.59	1.19
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	9	1.15	0.2	1.12
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	9	1.15	0.2	1.12
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	9	1.15	0.2	1.12
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	9	1.14	0.84	1.17
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	9	1.09	0.65	0.93

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	9	1.09	0.65	0.93
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	9	1.09	0.65	0.93
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	9	1.09	0.41	1.14
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	9	1.09	0.41	1.14
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	9	1.09	0.41	1.14
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	9	0.97	0.28	0.85
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	9	0.97	0.28	0.85
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	9	0.97	0.28	0.85
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD11	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD12	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD13	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD11	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD12	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD13	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD11	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD12	9	0.93	0.41	0.81
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD13	9	0.93	0.41	0.81
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD11	9	0.93	0.41	0.81
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD12	9	0.93	0.41	0.81
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD13	9	0.93	0.41	0.81
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	9	0.84	0.18	0.87
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	9	0.79	0.13	0.78
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	9	0.79	0.29	0.92
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	9	0.78	0.39	0.6
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	9	0.78	0.39	0.6
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	9	0.78	0.39	0.6
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	9	0.77	0.44	0.9
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	9	0.76	0.57	0.51
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	9	0.76	0.41	0.56
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	9	0.76	0.41	0.56
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	9	0.76	0.41	0.56
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	9	0.75	0.29	0.89
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	9	0.75	0.34	0.79
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	9	0.75	0.44	0.59
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	9	0.75	0.44	0.59
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	9	0.75	0.44	0.59
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	9	0.72	0.29	0.85
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	9	0.71	0.06	0.71
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	9	0.68	0.25	0.71
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	9	0.68	0.25	0.71
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	9	0.67	0.39	0.36
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	9	0.66	0.19	0.68

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	9	0.66	0.19	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	9	0.66	0.19	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	9	0.66	0.19	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	9	0.66	0.19	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	9	0.66	0.19	0.68
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	9	0.64	0.35	0.6
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	9	0.63	0.33	0.49
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	9	0.62	0.18	0.55
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	9	0.62	0.18	0.55
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	9	0.62	0.18	0.55
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	9	0.61	0.37	0.52
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	9	0.61	0.37	0.52
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	9	0.61	0.37	0.52
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	9	0.6	0.31	0.63
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	9	0.6	0.31	0.63
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	9	0.6	0.31	0.63
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	9	0.59	0.34	0.44
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	9	0.58	0.38	0.35
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	9	0.55	0.34	0.4
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	9	0.53	0.23	0.45
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	9	0.52	0.09	0.55
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	9	0.51	0.55	0.22
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	9	0.46	0.18	0.49
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	9	0.44	0.21	0.48
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	9	0.4	0.29	0.29
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	9	0.4	0.29	0.29
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	9	0.38	0.11	0.4
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	9	0.37	0.4	0.25
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	9	0.37	0.4	0.25
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	9	0.37	0.4	0.25
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	9	0.34	0.17	0.29
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	9	0.33	0.15	0.34
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	9	0.33	0.14	0.32
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	9	0.33	0.14	0.29
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	9	0.33	0.14	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	9	0.33	0.14	0.29
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	9	0.3	0.13	0.22
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	9	0.3	0.13	0.22
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	9	0.29	0.09	0.26
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	9	0.27	0.11	0.26
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	9	0.26	0.07	0.26
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	9	0.25	0.03	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	9	0.25	0.03	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	9	0.25	0.03	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	9	0.25	0.03	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	9	0.25	0.03	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	9	0.25	0.03	0.25
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	9	0.24	0.05	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	9	0.24	0.05	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	9	0.24	0.05	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	9	0.24	0.05	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	9	0.24	0.05	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	9	0.24	0.05	0.22
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	9	0.24	0.03	0.25
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	9	0.24	0.03	0.25
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	9	0.24	0.03	0.25
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	9	0.24	0.03	0.25
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	9	0.24	0.03	0.25
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	9	0.24	0.03	0.25
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	9	0.24	0.09	0.21
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	9	0.24	0.09	0.21
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	9	0.23	0.05	0.22
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	9	0.23	0.05	0.22
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	9	0.23	0.05	0.22
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	9	0.23	0.07	0.25
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	9	0.2	0.08	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	9	0.2	0.08	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	9	0.2	0.08	0.18
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	9	0.19	0.02	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	9	0.19	0.02	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	9	0.19	0.02	0.19
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	9	0.17	0.03	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	9	0.17	0.03	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	9	0.17	0.03	0.18
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	9	0.16	0.08	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	9	0.16	0.08	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	9	0.16	0.08	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	9	0.15	0.01	0.15
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	9	0.15	0.01	0.15
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	9	0.15	0.01	0.15
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	9	0.14	0.02	0.14
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	9	0.12	0.0	0.12
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	8	3.32	0.95	3.07
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	8	2.71	1.36	2.49
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	8	2.49	1.48	2.55
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	8	2.37	0.86	2.6
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	8	1.92	1.53	1.44
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	8	1.92	1.53	1.44
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	8	1.92	1.53	1.44
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	8	1.77	1.53	1.29
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	8	1.77	1.53	1.29
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	8	1.77	1.53	1.29
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	8	1.61	1.05	1.14
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	8	1.61	1.05	1.14
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	8	1.61	1.05	1.14
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	8	1.6	0.76	1.92
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	8	1.6	0.76	1.92
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	8	1.53	1.19	1.24
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	8	1.53	1.19	1.24
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	8	1.53	1.19	1.24
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	8	1.46	0.5	1.67
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	8	1.46	0.5	1.67
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	8	1.46	0.5	1.67
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	8	1.36	0.99	1.06
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	8	1.12	1.2	0.8
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	8	1.07	0.53	1.14
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	8	1.05	0.78	0.83
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	8	1.05	0.78	0.83
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	8	1.05	0.78	0.83
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	8	0.94	0.44	0.88
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	8	0.94	0.44	0.88
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	8	0.94	0.44	0.88
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	8	0.93	0.61	0.89
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	8	0.92	0.43	0.88
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	8	0.91	0.8	0.68
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	8	0.91	0.8	0.68
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	8	0.91	0.8	0.68
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	8	0.91	1.15	0.52

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	8	0.91	1.15	0.52
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	8	0.91	1.15	0.52
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	8	0.86	0.31	0.78
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	8	0.86	0.31	0.78
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	8	0.86	0.31	0.78
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	8	0.85	0.31	0.84
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	8	0.85	0.31	0.84
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	8	0.85	0.31	0.84
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	8	0.83	0.35	0.77
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	8	0.83	0.35	0.77
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	8	0.83	0.35	0.77
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	8	0.78	0.51	0.64
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	8	0.78	0.51	0.64
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	8	0.78	0.51	0.64
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	8	0.77	0.31	0.65
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	8	0.75	0.33	0.75
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	8	0.68	0.48	0.44
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	8	0.68	0.48	0.44
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	8	0.65	0.45	0.5
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	8	0.65	0.45	0.5
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	8	0.65	0.45	0.5

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	8	0.63	0.28	0.63
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	8	0.6	0.2	0.56
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	8	0.58	0.13	0.62
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	8	0.58	0.09	0.55
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	8	0.54	0.17	0.52
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	8	0.53	0.06	0.53
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	8	0.53	0.25	0.68
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	8	0.52	0.26	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	8	0.52	0.26	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	8	0.52	0.26	0.41
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	8	0.51	0.24	0.5
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	8	0.48	0.22	0.53
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	8	0.47	0.27	0.4
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	8	0.44	0.11	0.39
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	8	0.44	0.11	0.39
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	8	0.44	0.11	0.39
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	8	0.44	0.11	0.39
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	8	0.44	0.11	0.39
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	8	0.44	0.11	0.39
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	8	0.4	0.22	0.35
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	8	0.4	0.22	0.35
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	8	0.37	0.15	0.36
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	8	0.37	0.15	0.36
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	8	0.37	0.15	0.36
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	8	0.36	0.46	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	8	0.36	0.46	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	8	0.36	0.46	0.22
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	8	0.33	0.16	0.33
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	8	0.33	0.16	0.33
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	8	0.33	0.09	0.34
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	8	0.33	0.09	0.34
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	8	0.33	0.09	0.34
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	8	0.32	0.16	0.26
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	8	0.32	0.16	0.26
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	8	0.32	0.16	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	8	0.28	0.14	0.2
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	8	0.28	0.14	0.2
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	8	0.26	0.05	0.26
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	8	0.25	0.09	0.26
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	8	0.25	0.09	0.26
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	8	0.25	0.09	0.26
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	8	0.23	0.06	0.24
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	8	0.22	0.1	0.21
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	8	0.22	0.07	0.21
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	8	0.21	0.02	0.22
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	8	0.21	0.02	0.22
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	8	0.21	0.02	0.22
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	8	0.19	0.06	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	8	0.19	0.06	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	8	0.19	0.06	0.18
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	8	0.18	0.07	0.16
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	8	0.16	0.04	0.15
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	8	0.16	0.04	0.15
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	8	0.16	0.04	0.15
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	8	0.16	0.04	0.15
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	8	0.16	0.04	0.15
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	8	0.16	0.04	0.15
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	7	2.4	0.99	2.31
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	7	2.28	1.07	2.76
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	7	2.28	1.07	2.76
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	7	2.14	0.94	2.21
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	7	2.14	0.94	2.21
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	7	2.14	0.94	2.21
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	7	1.99	1.26	1.83
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	7	1.99	1.26	1.83
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	7	1.99	1.26	1.83
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	7	1.9	0.79	2.18
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	7	1.9	0.79	2.18
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	7	1.72	1.2	1.14
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	7	1.72	1.2	1.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	7	1.72	1.2	1.14
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	7	1.62	1.6	1.11
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	7	1.53	1.14	1.39
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	7	1.46	1.07	1.33
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	7	1.46	1.07	1.33
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	7	1.46	1.07	1.33
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	7	1.43	0.54	1.39
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	7	1.4	1.08	1.01
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	7	1.3	0.84	1.48
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	7	1.3	0.84	1.48
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	7	1.3	0.84	1.48
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	7	1.3	0.45	1.17
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	7	1.25	0.58	1.47
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	7	1.25	0.58	1.47
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	7	1.25	0.58	1.47
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	7	1.25	0.4	1.14
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	7	1.22	0.46	1.11
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	7	1.22	0.46	1.11
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	7	1.22	0.46	1.11
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	7	1.19	0.75	0.82
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	7	1.14	0.36	1.39
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	7	1.14	0.36	1.39
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	7	1.14	0.36	1.39
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	7	1.11	0.53	0.93
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	7	1.11	0.53	0.93
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	7	1.11	0.53	0.93
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	7	1.11	0.57	0.88
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	7	1.01	0.19	1.13
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	7	1.0	0.7	0.77
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	7	0.9	0.66	0.43
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	7	0.9	0.66	0.43
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	7	0.9	0.66	0.43
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	7	0.89	0.26	0.96
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	7	0.89	0.26	0.96
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	7	0.89	0.26	0.96
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	7	0.87	0.35	0.91
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	7	0.87	0.35	0.91
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	7	0.87	0.35	0.91
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	7	0.86	0.16	0.87
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	7	0.85	0.18	0.83
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	7	0.83	0.29	0.73
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	7	0.83	0.29	0.73

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	7	0.83	0.29	0.73
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	7	0.8	0.28	0.96
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	7	0.79	0.37	0.7
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	7	0.78	0.57	0.69
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	7	0.78	0.32	0.78
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	7	0.78	0.32	0.78
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	7	0.78	0.32	0.78
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	7	0.77	0.29	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	7	0.77	0.29	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	7	0.77	0.29	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	7	0.77	0.29	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	7	0.77	0.29	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	7	0.77	0.29	0.7
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	7	0.76	0.36	0.81
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	7	0.76	0.36	0.81
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	7	0.76	0.36	0.81
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	7	0.76	0.14	0.75
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	7	0.76	0.14	0.75
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	7	0.76	0.14	0.75
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	7	0.7	0.02	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	7	0.7	0.02	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	7	0.7	0.02	0.69
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	7	0.66	0.16	0.7
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	7	0.66	0.16	0.7
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	7	0.63	0.28	0.78
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	7	0.6	0.33	0.67
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	7	0.6	0.31	0.63
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	7	0.6	0.4	0.56
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	7	0.6	0.4	0.56
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	7	0.6	0.4	0.56
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	7	0.6	0.4	0.56
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	7	0.6	0.4	0.56
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	7	0.6	0.4	0.56
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	7	0.6	0.4	0.56
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	7	0.6	0.4	0.56

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	7	0.6	0.4	0.56
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	7	0.6	0.23	0.6
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	7	0.6	0.23	0.6
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	7	0.6	0.23	0.6
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	7	0.56	0.14	0.53
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	7	0.55	0.22	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	7	0.55	0.22	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	7	0.55	0.22	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	7	0.55	0.22	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	7	0.55	0.22	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	7	0.55	0.22	0.45
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	7	0.53	0.28	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	7	0.53	0.28	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	7	0.53	0.28	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	7	0.53	0.28	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	7	0.53	0.28	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	7	0.53	0.28	0.56
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	7	0.51	0.23	0.44
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	7	0.51	0.23	0.44
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	7	0.51	0.23	0.44
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	7	0.48	0.32	0.37
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	7	0.47	0.16	0.48
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	7	0.45	0.49	0.26
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	7	0.39	0.12	0.45
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	7	0.35	0.2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	7	0.35	0.2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	7	0.35	0.2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	7	0.35	0.2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	7	0.35	0.2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	7	0.35	0.2	0.27
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	7	0.34	0.12	0.4
(1,137)	1:56:A:SER:HB2	1:62:A:ASN:H	7	0.33	0.19	0.27
(1,137)	1:65:A:GLU:HA	1:62:A:ASN:H	7	0.33	0.19	0.27
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	7	0.3	0.14	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	7	0.3	0.14	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	7	0.3	0.14	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	7	0.3	0.14	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	7	0.3	0.14	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	7	0.3	0.14	0.3
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	7	0.29	0.12	0.3
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	7	0.29	0.12	0.3
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	7	0.29	0.12	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	7	0.25	0.14	0.16
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	7	0.25	0.14	0.16
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	7	0.25	0.14	0.16
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	7	0.24	0.04	0.25
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	7	0.24	0.04	0.25
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	7	0.23	0.01	0.23
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	7	0.23	0.01	0.23
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	7	0.23	0.01	0.23
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	7	0.23	0.1	0.22
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	7	0.22	0.09	0.16
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	7	0.22	0.09	0.16
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	7	0.21	0.06	0.24
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	7	0.19	0.03	0.2
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	7	0.18	0.04	0.17
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	7	0.17	0.04	0.19
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE1	6	2.75	1.13	2.62
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE2	6	2.75	1.13	2.62
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE3	6	2.75	1.13	2.62
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	6	2.32	1.5	2.12
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	6	2.32	1.5	2.12
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	6	2.32	1.5	2.12
(1,1874)	1:170:A:ARG:HE	1:177:A:THR:H	6	2.28	0.77	2.5
(1,3456)	1:158:A:HIS:HD2	1:94:A:VAL:HA	6	1.86	0.96	1.7
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	6	1.77	0.96	2.05
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	6	1.77	0.96	2.05
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	6	1.77	0.96	2.05
(1,307)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	6	1.76	1.0	2.32
(1,307)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	6	1.76	1.0	2.32
(1,307)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	6	1.76	1.0	2.32
(1,2771)	1:137:A:SER:HA	1:119:A:SER:H	6	1.62	1.15	1.31
(1,3311)	1:158:A:HIS:HD2	1:157:A:ILE:HG12	6	1.56	0.76	1.78
(1,1992)	1:92:A:SER:HB2	1:93:A:ASN:HD22	6	1.5	1.02	1.25
(1,1396)	1:158:A:HIS:HD2	1:154:A:ALA:HA	6	1.47	0.61	1.42
(1,2513)	1:142:A:LEU:HD21	1:139:A:ARG:H	6	1.42	0.92	1.65
(1,2513)	1:142:A:LEU:HD22	1:139:A:ARG:H	6	1.42	0.92	1.65

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2513)	1:142:A:LEU:HD23	1:139:A:ARG:H	6	1.42	0.92	1.65
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD11	6	1.21	0.78	0.94
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD12	6	1.21	0.78	0.94
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD13	6	1.21	0.78	0.94
(1,2701)	1:99:A:GLN:HE22	1:95:A:ARG:HG3	6	1.18	0.84	1.22
(1,524)	1:124:A:ASP:HB2	1:131:A:LEU:H	6	1.16	0.76	0.96
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG11	6	1.14	0.05	1.15
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG12	6	1.14	0.05	1.15
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG13	6	1.14	0.05	1.15
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	6	1.14	0.81	0.96
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	6	1.14	0.81	0.96
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	6	1.14	0.81	0.96
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD1	6	1.09	0.58	1.03
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD2	6	1.09	0.58	1.03
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD11	6	1.09	0.47	1.16
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD12	6	1.09	0.47	1.16
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD13	6	1.09	0.47	1.16
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD21	6	1.09	0.47	1.16
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD22	6	1.09	0.47	1.16
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD23	6	1.09	0.47	1.16
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	6	1.03	0.81	0.84
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	6	1.03	0.81	0.84
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	6	1.03	0.81	0.84
(1,525)	1:131:A:LEU:HB2	1:183:A:GLU:H	6	0.97	0.61	0.74
(1,3461)	1:132:A:ILE:HG12	1:125:A:ALA:H	6	0.93	0.51	1.02
(1,1810)	1:93:A:ASN:HD22	1:96:A:GLU:HB3	6	0.92	0.49	0.82
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE1	6	0.9	0.61	0.8
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE2	6	0.9	0.61	0.8
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB1	6	0.89	0.42	0.8
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB2	6	0.89	0.42	0.8
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB3	6	0.89	0.42	0.8
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD21	6	0.78	0.38	0.7
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD22	6	0.78	0.38	0.7
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD23	6	0.78	0.38	0.7
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG21	6	0.78	0.45	0.68
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG22	6	0.78	0.45	0.68
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG23	6	0.78	0.45	0.68
(2,4)	1:139:A:ARG:HH21	2:201:A:Z90:OAB	6	0.77	0.31	0.79
(1,2552)	1:99:A:GLN:HE22	1:96:A:GLU:H	6	0.7	0.28	0.68
(1,1935)	1:135:A:TYR:HD1	1:119:A:SER:H	6	0.67	0.44	0.5
(1,1935)	1:135:A:TYR:HD2	1:119:A:SER:H	6	0.67	0.44	0.5
(1,82)	1:19:A:PRO:HG2	1:21:A:VAL:H	6	0.63	0.2	0.72

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,82)	1:19:A:PRO:HG3	1:21:A:VAL:H	6	0.63	0.2	0.72
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD11	6	0.61	0.28	0.58
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD12	6	0.61	0.28	0.58
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD13	6	0.61	0.28	0.58
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD21	6	0.61	0.31	0.6
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD22	6	0.61	0.31	0.6
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD23	6	0.61	0.31	0.6
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD11	6	0.61	0.14	0.58
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD12	6	0.61	0.14	0.58
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD13	6	0.61	0.14	0.58
(1,212)	1:162:A:ILE:HG21	1:182:A:GLU:H	6	0.61	0.14	0.58
(1,212)	1:162:A:ILE:HG22	1:182:A:GLU:H	6	0.61	0.14	0.58
(1,212)	1:162:A:ILE:HG23	1:182:A:GLU:H	6	0.61	0.14	0.58
(1,624)	1:92:A:SER:H	1:96:A:GLU:HG3	6	0.59	0.34	0.47
(1,401)	1:132:A:ILE:HA	1:125:A:ALA:H	6	0.58	0.25	0.55
(1,3297)	1:143:A:GLN:HE22	1:142:A:LEU:H	6	0.57	0.34	0.55
(1,864)	1:166:A:VAL:HB	1:178:A:GLN:H	6	0.57	0.16	0.58
(1,3354)	1:27:A:LYS:HD3	1:28:A:GLU:H	6	0.56	0.31	0.64
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD11	6	0.56	0.02	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD12	6	0.56	0.02	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD13	6	0.56	0.02	0.56
(1,1156)	1:100:A:ASN:HB3	1:99:A:GLN:H	6	0.56	0.13	0.55
(1,1988)	1:26:A:LYS:HB3	1:23:A:GLU:H	6	0.55	0.69	0.26
(1,2577)	1:128:A:GLY:HA3	1:130:A:GLY:H	6	0.52	0.23	0.55
(1,2786)	1:14:A:ILE:HG13	1:22:A:TRP:HE1	6	0.51	0.34	0.36
(1,2863)	1:126:A:GLU:H	1:130:A:GLY:H	6	0.48	0.34	0.4
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD21	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD22	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD23	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD21	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD22	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD23	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD21	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD22	6	0.44	0.13	0.44
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD23	6	0.44	0.13	0.44
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD21	6	0.43	0.11	0.45
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD22	6	0.43	0.11	0.45
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD23	6	0.43	0.11	0.45
(1,1960)	1:184:A:LYS:HE2	1:184:A:LYS:HA	6	0.42	0.23	0.3
(1,2273)	1:11:A:LEU:HB3	1:8:A:ALA:H	6	0.39	0.14	0.36
(1,2042)	1:176:A:HIS:H	1:174:A:CYS:H	6	0.36	0.12	0.34
(1,601)	1:170:A:ARG:HG2	1:171:A:ASN:H	6	0.35	0.1	0.36

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2961)	1:123:A:THR:HB	1:124:A:ASP:H	6	0.34	0.13	0.37
(1,1053)	1:162:A:ILE:HA	1:164:A:MET:H	6	0.34	0.22	0.22
(1,2466)	1:95:A:ARG:H	1:93:A:ASN:H	6	0.33	0.15	0.3
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD11	6	0.32	0.23	0.2
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD12	6	0.32	0.23	0.2
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD13	6	0.32	0.23	0.2
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD11	6	0.32	0.2	0.29
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD12	6	0.32	0.2	0.29
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD13	6	0.32	0.2	0.29
(1,2118)	1:94:A:VAL:HG21	1:96:A:GLU:H	6	0.31	0.13	0.24
(1,2118)	1:94:A:VAL:HG22	1:96:A:GLU:H	6	0.31	0.13	0.24
(1,2118)	1:94:A:VAL:HG23	1:96:A:GLU:H	6	0.31	0.13	0.24
(1,2930)	1:61:A:LEU:HD11	1:66:A:ILE:H	6	0.28	0.13	0.24
(1,2930)	1:61:A:LEU:HD12	1:66:A:ILE:H	6	0.28	0.13	0.24
(1,2930)	1:61:A:LEU:HD13	1:66:A:ILE:H	6	0.28	0.13	0.24
(1,3289)	1:63:A:ALA:HB1	1:67:A:LEU:H	6	0.26	0.09	0.28
(1,3289)	1:63:A:ALA:HB2	1:67:A:LEU:H	6	0.26	0.09	0.28
(1,3289)	1:63:A:ALA:HB3	1:67:A:LEU:H	6	0.26	0.09	0.28
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD11	6	0.23	0.02	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD12	6	0.23	0.02	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD13	6	0.23	0.02	0.23
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG21	6	0.22	0.07	0.19
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG22	6	0.22	0.07	0.19
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG23	6	0.22	0.07	0.19
(1,2155)	1:125:A:ALA:HA	1:126:A:GLU:H	6	0.16	0.04	0.15
(1,622)	1:140:A:GLU:HB3	1:170:A:ARG:H	5	2.69	1.34	3.31
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE1	5	2.32	0.85	2.26
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE2	5	2.32	0.85	2.26
(1,2460)	1:138:A:GLU:H	1:118:A:PRO:HA	5	2.31	0.78	2.41
(1,254)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	5	1.81	0.74	2.04
(1,254)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	5	1.81	0.74	2.04
(1,254)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	5	1.81	0.74	2.04
(1,1146)	1:100:A:ASN:HD22	1:99:A:GLN:H	5	1.75	1.18	2.6
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD11	5	1.72	0.98	1.63
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD12	5	1.72	0.98	1.63
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD13	5	1.72	0.98	1.63
(1,2125)	1:136:A:TYR:HA	1:119:A:SER:H	5	1.62	0.89	1.47
(1,2301)	1:136:A:TYR:HA	1:119:A:SER:H	5	1.61	0.89	1.47
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	5	1.43	0.66	1.55
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	5	1.43	0.66	1.55
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	5	1.43	0.66	1.55
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG11	5	1.4	0.78	1.87

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG12	5	1.4	0.78	1.87
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG13	5	1.4	0.78	1.87
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG11	5	1.4	0.78	1.87
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG12	5	1.4	0.78	1.87
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG13	5	1.4	0.78	1.87
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG11	5	1.4	0.78	1.87
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG12	5	1.4	0.78	1.87
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG13	5	1.4	0.78	1.87
(1,2007)	1:69:A:MET:HG2	1:67:A:LEU:H	5	1.32	0.18	1.27
(1,1187)	1:31:A:LEU:HA	1:35:A:GLY:H	5	1.26	0.62	1.27
(1,1439)	1:99:A:GLN:HE22	1:95:A:ARG:HG2	5	1.23	0.62	1.58
(1,316)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	5	1.16	0.43	1.13
(1,316)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	5	1.16	0.43	1.13
(1,316)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	5	1.16	0.43	1.13
(1,2188)	1:183:A:GLU:HB2	1:185:A:GLU:H	5	1.12	0.7	0.77
(1,2086)	1:93:A:ASN:HD22	1:96:A:GLU:H	5	1.09	0.45	1.25
(1,2634)	1:173:A:GLU:HG3	1:172:A:GLU:H	5	1.08	0.35	1.15
(1,1956)	1:34:A:GLU:HB2	1:36:A:GLN:H	5	1.05	0.63	0.94
(1,1956)	1:34:A:GLU:HB3	1:36:A:GLN:H	5	1.05	0.63	0.94
(1,265)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	5	1.04	0.43	1.01
(1,265)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	5	1.04	0.43	1.01
(1,265)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	5	1.04	0.43	1.01
(1,2266)	1:171:A:ASN:HD22	1:173:A:GLU:H	5	1.04	0.18	1.01
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD11	5	1.04	1.02	0.32
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD12	5	1.04	1.02	0.32
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD13	5	1.04	1.02	0.32
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD11	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD12	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD13	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD11	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD12	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD13	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD11	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD12	5	0.92	0.52	0.92
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD13	5	0.92	0.52	0.92
(1,1529)	1:93:A:ASN:HD22	1:93:A:ASN:H	5	0.9	0.58	1.33
(1,1066)	1:139:A:ARG:HG3	1:140:A:GLU:H	5	0.87	0.53	1.22
(1,574)	1:120:A:PHE:H	1:121:A:ARG:HB3	5	0.84	0.37	0.96
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG21	5	0.84	0.35	0.74
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG22	5	0.84	0.35	0.74
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG23	5	0.84	0.35	0.74
(1,3384)	1:120:A:PHE:HD1	1:135:A:TYR:H	5	0.81	0.23	0.78

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3384)	1:120:A:PHE:HD2	1:135:A:TYR:H	5	0.81	0.23	0.78
(1,1985)	1:136:A:TYR:HD1	1:135:A:TYR:H	5	0.8	0.46	0.94
(1,1985)	1:136:A:TYR:HD2	1:135:A:TYR:H	5	0.8	0.46	0.94
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD21	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD22	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD23	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD21	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD22	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD23	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD21	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD22	5	0.78	0.41	0.72
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD23	5	0.78	0.41	0.72
(1,593)	1:170:A:ARG:HG3	1:171:A:ASN:H	5	0.77	0.06	0.77
(1,1951)	1:184:A:LYS:HE3	1:184:A:LYS:HA	5	0.74	0.22	0.81
(1,2196)	1:164:A:MET:HA	1:165:A:LYS:HD2	5	0.71	0.33	0.73
(1,548)	1:143:A:GLN:HE22	1:144:A:ASP:H	5	0.7	0.32	0.7
(1,462)	1:165:A:LYS:HD3	1:180:A:LEU:H	5	0.66	0.23	0.76
(1,2795)	1:16:A:ASN:HD22	1:16:A:ASN:H	5	0.65	0.41	0.43
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD21	5	0.61	0.34	0.49
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD22	5	0.61	0.34	0.49
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD23	5	0.61	0.34	0.49
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD21	5	0.6	0.2	0.58
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD22	5	0.6	0.2	0.58
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD23	5	0.6	0.2	0.58
(1,1725)	1:128:A:GLY:H	1:130:A:GLY:H	5	0.6	0.37	0.43
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG21	5	0.58	0.4	0.4
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG22	5	0.58	0.4	0.4
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG23	5	0.58	0.4	0.4
(1,1459)	1:79:A:GLN:HB2	1:82:A:GLY:H	5	0.58	0.19	0.59
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG21	5	0.56	0.39	0.36
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG22	5	0.56	0.39	0.36
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG23	5	0.56	0.39	0.36
(1,120)	1:27:A:LYS:HD2	1:30:A:GLN:H	5	0.54	0.41	0.34
(1,120)	1:27:A:LYS:HD3	1:30:A:GLN:H	5	0.54	0.41	0.34
(1,2415)	1:75:A:PHE:HE1	1:156:A:GLN:H	5	0.53	0.23	0.51
(1,2415)	1:75:A:PHE:HE2	1:156:A:GLN:H	5	0.53	0.23	0.51
(1,1495)	1:125:A:ALA:HB1	1:131:A:LEU:H	5	0.53	0.3	0.48
(1,1495)	1:125:A:ALA:HB2	1:131:A:LEU:H	5	0.53	0.3	0.48
(1,1495)	1:125:A:ALA:HB3	1:131:A:LEU:H	5	0.53	0.3	0.48
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD21	5	0.51	0.38	0.54
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD22	5	0.51	0.38	0.54
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD23	5	0.51	0.38	0.54

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD21	5	0.51	0.38	0.54
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD22	5	0.51	0.38	0.54
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD23	5	0.51	0.38	0.54
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD21	5	0.51	0.38	0.54
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD22	5	0.51	0.38	0.54
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD23	5	0.51	0.38	0.54
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	5	0.5	0.52	0.21
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	5	0.5	0.52	0.21
(1,892)	1:172:A:GLU:H	1:171:A:ASN:HD22	5	0.49	0.17	0.54
(1,3573)	1:22:A:TRP:HE3	1:26:A:LYS:HB2	5	0.49	0.61	0.24
(1,2720)	1:140:A:GLU:HG2	1:142:A:LEU:H	5	0.49	0.26	0.45
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG21	5	0.46	0.25	0.48
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG22	5	0.46	0.25	0.48
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG23	5	0.46	0.25	0.48
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD21	5	0.46	0.11	0.47
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD22	5	0.46	0.11	0.47
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD23	5	0.46	0.11	0.47
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD11	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD12	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD13	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD11	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD12	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD13	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD11	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD12	5	0.44	0.19	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD13	5	0.44	0.19	0.31
(1,2394)	1:17:A:TYR:HE1	1:13:A:VAL:H	5	0.44	0.15	0.5
(1,2394)	1:17:A:TYR:HE2	1:13:A:VAL:H	5	0.44	0.15	0.5
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG21	5	0.44	0.15	0.49
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG22	5	0.44	0.15	0.49
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG23	5	0.44	0.15	0.49
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG21	5	0.44	0.35	0.34
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG22	5	0.44	0.35	0.34
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG23	5	0.44	0.35	0.34
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE1	5	0.43	0.25	0.46

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE2	5	0.43	0.25	0.46
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE1	5	0.43	0.25	0.46
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE2	5	0.43	0.25	0.46
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE1	5	0.43	0.25	0.46
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE2	5	0.43	0.25	0.46
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD11	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD12	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD13	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD11	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD12	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD13	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD11	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD12	5	0.42	0.38	0.23
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD13	5	0.42	0.38	0.23
(1,334)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	5	0.41	0.14	0.42
(1,334)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	5	0.41	0.14	0.42
(1,334)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	5	0.41	0.14	0.42
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD11	5	0.39	0.2	0.4
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD12	5	0.39	0.2	0.4
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD13	5	0.39	0.2	0.4
(1,614)	1:170:A:ARG:HG2	1:170:A:ARG:H	5	0.37	0.09	0.38
(1,148)	1:145:A:ILE:HG12	1:143:A:GLN:H	5	0.35	0.1	0.33
(1,148)	1:145:A:ILE:HG13	1:143:A:GLN:H	5	0.35	0.1	0.33
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG11	5	0.34	0.17	0.34
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG12	5	0.34	0.17	0.34
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG13	5	0.34	0.17	0.34
(1,1817)	1:66:A:ILE:HB	1:56:A:SER:H	5	0.34	0.25	0.19
(1,670)	1:143:A:GLN:HG3	1:142:A:LEU:H	5	0.33	0.1	0.29
(1,2673)	1:34:A:GLU:HA	1:35:A:GLY:H	5	0.3	0.06	0.33
(1,2436)	1:66:A:ILE:HG12	1:56:A:SER:H	5	0.3	0.08	0.29
(1,576)	1:171:A:ASN:H	1:169:A:GLN:HA	5	0.3	0.05	0.3
(1,3197)	1:139:A:ARG:HG2	1:140:A:GLU:H	5	0.29	0.09	0.29
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG12	5	0.29	0.09	0.31
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG13	5	0.29	0.09	0.31
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD11	5	0.28	0.17	0.2
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD12	5	0.28	0.17	0.2
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD13	5	0.28	0.17	0.2
(1,1152)	1:62:A:ASN:HD22	1:63:A:ALA:H	5	0.27	0.05	0.29
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD21	5	0.25	0.05	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD22	5	0.25	0.05	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD23	5	0.25	0.05	0.24
(1,1345)	1:19:A:PRO:HD2	1:18:A:GLY:H	5	0.25	0.05	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3540)	1:54:A:ALA:HB1	1:28:A:GLU:H	5	0.24	0.12	0.21
(1,3540)	1:54:A:ALA:HB2	1:28:A:GLU:H	5	0.24	0.12	0.21
(1,3540)	1:54:A:ALA:HB3	1:28:A:GLU:H	5	0.24	0.12	0.21
(1,1502)	1:57:A:LYS:HG2	1:58:A:VAL:H	5	0.24	0.06	0.23
(1,818)	1:114:A:GLY:H	1:115:A:MET:H	5	0.24	0.06	0.23
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD11	5	0.22	0.07	0.24
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD12	5	0.22	0.07	0.24
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD13	5	0.22	0.07	0.24
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB1	5	0.2	0.1	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB2	5	0.2	0.1	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB3	5	0.2	0.1	0.13
(1,1582)	1:164:A:MET:HE1	1:181:A:ILE:HB	5	0.18	0.05	0.18
(1,1582)	1:164:A:MET:HE2	1:181:A:ILE:HB	5	0.18	0.05	0.18
(1,1582)	1:164:A:MET:HE3	1:181:A:ILE:HB	5	0.18	0.05	0.18
(1,3099)	1:8:A:ALA:HB1	1:12:A:LEU:H	5	0.15	0.06	0.12
(1,3099)	1:8:A:ALA:HB2	1:12:A:LEU:H	5	0.15	0.06	0.12
(1,3099)	1:8:A:ALA:HB3	1:12:A:LEU:H	5	0.15	0.06	0.12
(1,1014)	1:174:A:CYS:HB2	1:169:A:GLN:H	4	2.27	0.55	2.22
(1,2485)	1:30:A:GLN:HE22	1:28:A:GLU:HA	4	1.84	0.04	1.85
(1,998)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	4	1.83	1.14	1.98
(1,1565)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	4	1.77	1.14	1.92
(1,1704)	1:184:A:LYS:HD2	1:161:A:GLU:H	4	1.67	0.5	1.88
(1,1704)	1:184:A:LYS:HD3	1:161:A:GLU:H	4	1.67	0.5	1.88
(1,2316)	1:171:A:ASN:HB2	1:174:A:CYS:HB3	4	1.61	0.65	1.81
(1,2017)	1:136:A:TYR:HB2	1:119:A:SER:H	4	1.61	1.72	0.81
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE1	4	1.55	1.25	1.34
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE2	4	1.55	1.25	1.34
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE3	4	1.55	1.25	1.34
(1,1927)	1:120:A:PHE:HE1	1:119:A:SER:H	4	1.52	0.81	1.42
(1,1927)	1:120:A:PHE:HE2	1:119:A:SER:H	4	1.52	0.81	1.42
(1,2479)	1:92:A:SER:HB3	1:93:A:ASN:HD22	4	1.49	0.5	1.6
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD11	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD12	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD13	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD11	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD12	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD13	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD11	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD12	4	1.45	0.6	1.67
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD13	4	1.45	0.6	1.67
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD11	4	1.44	0.38	1.38
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD12	4	1.44	0.38	1.38

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD13	4	1.44	0.38	1.38
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD21	4	1.44	0.38	1.38
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD22	4	1.44	0.38	1.38
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD23	4	1.44	0.38	1.38
(1,420)	1:136:A:TYR:HB3	1:119:A:SER:H	4	1.42	1.01	1.32
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG21	4	1.34	1.13	1.2
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG22	4	1.34	1.13	1.2
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG23	4	1.34	1.13	1.2
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG21	4	1.34	1.13	1.2
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG22	4	1.34	1.13	1.2
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG23	4	1.34	1.13	1.2
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD21	4	1.33	0.74	1.48
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD22	4	1.33	0.74	1.48
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD23	4	1.33	0.74	1.48
(1,3098)	1:69:A:MET:HG3	1:73:A:MET:H	4	1.33	0.17	1.3
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	4	1.32	0.57	1.59
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	4	1.32	0.57	1.59
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	4	1.32	0.57	1.59
(1,3234)	1:100:A:ASN:HD22	1:96:A:GLU:HB3	4	1.28	0.72	1.38
(1,2503)	1:30:A:GLN:HE22	1:30:A:GLN:H	4	1.26	0.21	1.3
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD21	4	1.22	0.09	1.23
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD22	4	1.22	0.09	1.23
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD23	4	1.22	0.09	1.23
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD21	4	1.2	1.02	0.74
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD22	4	1.2	1.02	0.74
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD23	4	1.2	1.02	0.74
(1,2492)	1:99:A:GLN:HB2	1:98:A:LEU:H	4	1.14	0.61	1.4
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD11	4	1.12	0.74	0.84
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD12	4	1.12	0.74	0.84
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD13	4	1.12	0.74	0.84
(1,2340)	1:139:A:ARG:HG2	1:141:A:GLY:H	4	1.11	0.57	0.89
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD21	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD22	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD23	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD21	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD22	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD23	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD21	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD22	4	1.08	0.71	1.02
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD23	4	1.08	0.71	1.02
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD11	4	0.98	0.74	1.01
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD12	4	0.98	0.74	1.01

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD13	4	0.98	0.74	1.01
(1,1123)	1:94:A:VAL:HB	1:160:A:THR:HB	4	0.95	0.47	1.0
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD21	4	0.94	0.49	0.8
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD22	4	0.94	0.49	0.8
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD23	4	0.94	0.49	0.8
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD21	4	0.94	0.49	0.8
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD22	4	0.94	0.49	0.8
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD23	4	0.94	0.49	0.8
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	4	0.92	0.6	0.88
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	4	0.92	0.6	0.88
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	4	0.92	0.6	0.88
(1,1617)	1:49:A:TYR:HE1	1:48:A:THR:H	4	0.92	1.01	0.4
(1,1617)	1:49:A:TYR:HE2	1:48:A:THR:H	4	0.92	1.01	0.4
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD1	4	0.89	0.2	0.9
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD2	4	0.89	0.2	0.9
(1,1738)	1:176:A:HIS:HD2	1:135:A:TYR:H	4	0.85	0.51	0.92
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG11	4	0.82	0.14	0.82
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG12	4	0.82	0.14	0.82
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG13	4	0.82	0.14	0.82
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB2	4	0.79	0.28	0.73
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB3	4	0.79	0.28	0.73
(1,335)	1:101:A:LEU:HD11	2:201:A:Z90:HAH	4	0.76	0.17	0.8
(1,335)	1:101:A:LEU:HD12	2:201:A:Z90:HAH	4	0.76	0.17	0.8
(1,335)	1:101:A:LEU:HD13	2:201:A:Z90:HAH	4	0.76	0.17	0.8
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG21	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG22	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG23	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG21	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG22	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG23	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG21	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG22	4	0.75	0.25	0.78
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG23	4	0.75	0.25	0.78
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD2	4	0.72	0.44	0.8
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD3	4	0.72	0.44	0.8
(1,579)	1:173:A:GLU:HB2	1:171:A:ASN:H	4	0.72	0.51	0.62
(1,3565)	1:131:A:LEU:HG	1:181:A:ILE:H	4	0.72	0.5	0.68
(1,2871)	1:181:A:ILE:H	1:130:A:GLY:H	4	0.69	0.17	0.67
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG11	4	0.68	0.48	0.52
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG12	4	0.68	0.48	0.52
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG13	4	0.68	0.48	0.52
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG11	4	0.68	0.48	0.52

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG12	4	0.68	0.48	0.52
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG13	4	0.68	0.48	0.52
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG11	4	0.68	0.48	0.52
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG12	4	0.68	0.48	0.52
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG13	4	0.68	0.48	0.52
(1,454)	1:176:A:HIS:H	1:170:A:ARG:HA	4	0.68	0.17	0.7
(1,3133)	1:60:A:ASN:HD22	1:60:A:ASN:H	4	0.68	0.05	0.7
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD21	4	0.67	0.13	0.7
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD22	4	0.67	0.13	0.7
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD23	4	0.67	0.13	0.7
(1,3484)	1:37:A:PHE:H	1:35:A:GLY:H	4	0.65	0.22	0.68
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB2	4	0.64	0.32	0.77
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB3	4	0.64	0.32	0.77
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	4	0.64	0.19	0.7
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	4	0.64	0.19	0.7
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	4	0.64	0.19	0.7
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG21	4	0.62	0.29	0.69
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG22	4	0.62	0.29	0.69
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG23	4	0.62	0.29	0.69
(1,301)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	4	0.62	0.01	0.62
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB1	4	0.6	0.32	0.52

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB1	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB2	4	0.6	0.32	0.52
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB3	4	0.6	0.32	0.52
(1,2681)	1:181:A:ILE:HB	1:183:A:GLU:H	4	0.59	0.47	0.36
(1,935)	1:125:A:ALA:HA	1:132:A:ILE:HB	4	0.56	0.4	0.43
(1,645)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	4	0.55	0.18	0.57
(1,3353)	1:91:A:GLY:H	1:93:A:ASN:H	4	0.52	0.41	0.36
(1,2011)	1:30:A:GLN:HE22	1:30:A:GLN:HA	4	0.48	0.18	0.56
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE1	4	0.42	0.15	0.41
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE2	4	0.42	0.15	0.41
(1,3216)	1:27:A:LYS:HG2	1:27:A:LYS:H	4	0.42	0.02	0.42
(1,2838)	1:132:A:ILE:HG13	1:133:A:LEU:H	4	0.42	0.05	0.42
(1,2624)	1:173:A:GLU:HG2	1:172:A:GLU:H	4	0.42	0.15	0.42
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD11	4	0.42	0.13	0.45
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD12	4	0.42	0.13	0.45
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD13	4	0.42	0.13	0.45
(1,2884)	1:131:A:LEU:HB3	1:130:A:GLY:H	4	0.38	0.14	0.36
(1,3284)	1:100:A:ASN:HB3	1:103:A:ALA:H	4	0.38	0.22	0.32
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE1	4	0.38	0.3	0.24
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE2	4	0.38	0.3	0.24
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE3	4	0.38	0.3	0.24
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD21	4	0.37	0.1	0.38
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD22	4	0.37	0.1	0.38
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD23	4	0.37	0.1	0.38
(1,1297)	1:145:A:ILE:HG12	1:71:A:GLY:H	4	0.37	0.23	0.29
(1,311)	1:39:A:VAL:HG11	2:201:A:Z90:HAE	4	0.36	0.18	0.36
(1,311)	1:39:A:VAL:HG12	2:201:A:Z90:HAE	4	0.36	0.18	0.36
(1,311)	1:39:A:VAL:HG13	2:201:A:Z90:HAE	4	0.36	0.18	0.36
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD11	4	0.36	0.12	0.34
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD12	4	0.36	0.12	0.34
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD13	4	0.36	0.12	0.34
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD21	4	0.36	0.12	0.34
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD22	4	0.36	0.12	0.34
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD23	4	0.36	0.12	0.34
(1,798)	1:183:A:GLU:HA	1:162:A:ILE:HA	4	0.35	0.06	0.38
(1,467)	1:122:A:CYS:HB3	1:134:A:HIS:H	4	0.35	0.06	0.34
(1,262)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	4	0.34	0.01	0.34
(1,261)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	4	0.32	0.12	0.32
(1,596)	1:170:A:ARG:HG3	1:170:A:ARG:H	4	0.32	0.03	0.32
(1,1138)	1:73:A:MET:HE1	1:16:A:ASN:H	4	0.32	0.16	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1138)	1:73:A:MET:HE2	1:16:A:ASN:H	4	0.32	0.16	0.26
(1,1138)	1:73:A:MET:HE3	1:16:A:ASN:H	4	0.32	0.16	0.26
(1,874)	1:52:A:VAL:HB	1:67:A:LEU:H	4	0.32	0.06	0.33
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG11	4	0.31	0.08	0.3
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG12	4	0.31	0.08	0.3
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG13	4	0.31	0.08	0.3
(1,105)	1:182:A:GLU:H	1:164:A:MET:H	4	0.31	0.11	0.34
(1,105)	1:165:A:LYS:H	1:182:A:GLU:H	4	0.31	0.11	0.34
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	4	0.3	0.02	0.3
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	4	0.3	0.02	0.3
(1,971)	1:92:A:SER:HB3	1:93:A:ASN:H	4	0.3	0.03	0.31
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD11	4	0.3	0.05	0.31
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD12	4	0.3	0.05	0.31
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD13	4	0.3	0.05	0.31
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD21	4	0.3	0.05	0.31
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD22	4	0.3	0.05	0.31
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD23	4	0.3	0.05	0.31
(1,260)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	4	0.3	0.0	0.3
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE1	4	0.3	0.03	0.3
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE2	4	0.3	0.03	0.3
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE3	4	0.3	0.03	0.3
(1,50)	1:65:A:GLU:HA	1:69:A:MET:HE1	4	0.3	0.03	0.3
(1,50)	1:65:A:GLU:HA	1:69:A:MET:HE2	4	0.3	0.03	0.3
(1,50)	1:65:A:GLU:HA	1:69:A:MET:HE3	4	0.3	0.03	0.3
(1,1733)	1:49:A:TYR:HD1	1:142:A:LEU:H	4	0.29	0.13	0.3
(1,1733)	1:49:A:TYR:HD2	1:142:A:LEU:H	4	0.29	0.13	0.3
(1,2005)	1:47:A:LYS:HE3	1:47:A:LYS:H	4	0.28	0.11	0.3
(1,649)	1:33:A:GLU:H	1:31:A:LEU:H	4	0.28	0.11	0.26
(1,1984)	1:35:A:GLY:HA2	1:36:A:GLN:H	4	0.26	0.02	0.26
(1,99)	1:125:A:ALA:HA	1:132:A:ILE:H	4	0.26	0.1	0.24
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	4	0.26	0.02	0.26
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	4	0.26	0.02	0.26
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	4	0.26	0.02	0.26
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	4	0.26	0.02	0.26
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	4	0.26	0.02	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	4	0.26	0.02	0.26
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	4	0.26	0.02	0.26
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	4	0.26	0.02	0.26
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	4	0.26	0.02	0.26
(1,767)	1:66:A:ILE:HG12	1:61:A:LEU:H	4	0.26	0.19	0.17
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD11	4	0.26	0.07	0.29
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD12	4	0.26	0.07	0.29
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD13	4	0.26	0.07	0.29
(1,3183)	1:175:A:ASP:H	1:174:A:CYS:HB2	4	0.25	0.11	0.23
(1,948)	1:50:A:ASP:HB2	1:53:A:ALA:H	4	0.22	0.07	0.22
(1,2130)	1:167:A:ILE:HG12	1:179:A:PHE:H	4	0.22	0.09	0.23
(1,2171)	1:17:A:TYR:HD1	1:13:A:VAL:HA	4	0.21	0.02	0.2
(1,2171)	1:17:A:TYR:HD2	1:13:A:VAL:HA	4	0.21	0.02	0.2
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD21	4	0.2	0.07	0.2
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD22	4	0.2	0.07	0.2
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD23	4	0.2	0.07	0.2
(1,300)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	4	0.2	0.0	0.2
(1,161)	1:171:A:ASN:HD22	1:171:A:ASN:H	4	0.2	0.06	0.2
(1,161)	1:176:A:HIS:H	1:171:A:ASN:H	4	0.2	0.06	0.2
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG21	4	0.2	0.04	0.2
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG22	4	0.2	0.04	0.2
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG23	4	0.2	0.04	0.2
(1,1901)	1:131:A:LEU:HG	1:131:A:LEU:H	4	0.2	0.03	0.19
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG21	4	0.19	0.08	0.15
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG22	4	0.19	0.08	0.15
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG23	4	0.19	0.08	0.15
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB1	4	0.18	0.08	0.16
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB2	4	0.18	0.08	0.16
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB3	4	0.18	0.08	0.16
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB1	4	0.18	0.06	0.16
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB2	4	0.18	0.06	0.16
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB3	4	0.18	0.06	0.16
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD11	4	0.17	0.03	0.18
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD12	4	0.17	0.03	0.18
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD13	4	0.17	0.03	0.18
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD11	4	0.16	0.02	0.16
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD12	4	0.16	0.02	0.16
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD13	4	0.16	0.02	0.16
(1,2247)	1:174:A:CYS:H	1:174:A:CYS:HB3	4	0.15	0.05	0.13
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG12	4	0.14	0.03	0.13
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG13	4	0.14	0.03	0.13
(1,3402)	1:49:A:TYR:HA	1:48:A:THR:H	4	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)
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD1	3	3.07	1.5	2.59
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD2	3	3.07	1.5	2.59
(1,1019)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	3	2.2	0.77	2.47
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	3	1.73	0.83	2.02
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	3	1.73	0.83	2.02
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	3	1.73	0.83	2.02
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE1	3	1.58	0.96	2.2
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE2	3	1.58	0.96	2.2
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE3	3	1.58	0.96	2.2
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD1	3	1.57	0.82	1.07
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD2	3	1.57	0.82	1.07
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD1	3	1.57	0.82	1.07
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD2	3	1.57	0.82	1.07
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD1	3	1.57	0.82	1.07
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD2	3	1.57	0.82	1.07
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG21	3	1.57	0.59	1.43
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG22	3	1.57	0.59	1.43
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG23	3	1.57	0.59	1.43
(1,558)	1:125:A:ALA:HA	1:132:A:ILE:HG13	3	1.48	0.94	1.2
(2,1)	1:135:A:TYR:HH	2:201:A:Z90:OAC	3	1.46	0.9	0.94
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD21	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD22	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD23	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD21	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD22	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD23	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD21	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD22	3	1.42	0.51	1.42
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD23	3	1.42	0.51	1.42
(1,1494)	1:176:A:HIS:H	1:174:A:CYS:HB2	3	1.39	0.82	1.97
(1,450)	1:155:A:GLN:HG3	1:159:A:GLY:H	3	1.37	1.12	0.94
(1,3044)	1:136:A:TYR:HD1	1:119:A:SER:H	3	1.34	1.48	0.45
(1,3044)	1:136:A:TYR:HD2	1:119:A:SER:H	3	1.34	1.48	0.45
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE1	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE2	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE3	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE1	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE2	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE3	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE1	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE2	3	1.28	0.48	1.46
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE3	3	1.28	0.48	1.46

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG11	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG12	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG13	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG11	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG12	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG13	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG11	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG12	3	1.23	0.11	1.17
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG13	3	1.23	0.11	1.17
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG11	3	1.1	0.64	0.87
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG12	3	1.1	0.64	0.87
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG13	3	1.1	0.64	0.87
(1,3526)	1:12:A:LEU:HA	1:16:A:ASN:HD22	3	1.03	0.58	0.8
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD11	3	1.02	0.36	0.87
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD12	3	1.02	0.36	0.87
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD13	3	1.02	0.36	0.87
(1,2169)	1:186:A:SER:H	1:184:A:LYS:HA	3	1.0	0.78	0.88
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG11	3	0.99	0.06	1.01
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG12	3	0.99	0.06	1.01
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG13	3	0.99	0.06	1.01
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG11	3	0.99	0.06	1.01
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG12	3	0.99	0.06	1.01
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG13	3	0.99	0.06	1.01
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD2	3	0.99	0.57	1.25
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD3	3	0.99	0.57	1.25
(1,3107)	1:24:A:ASP:HB3	1:22:A:TRP:H	3	0.98	0.17	1.09
(1,2995)	1:176:A:HIS:HA	1:137:A:SER:H	3	0.98	0.6	1.26
(1,2116)	1:161:A:GLU:HG3	1:160:A:THR:HA	3	0.96	0.39	1.23
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG11	3	0.96	0.05	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG12	3	0.96	0.05	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG13	3	0.96	0.05	0.92
(1,40)	1:57:A:LYS:HB2	1:58:A:VAL:HG11	3	0.96	0.05	0.92
(1,40)	1:57:A:LYS:HB2	1:58:A:VAL:HG12	3	0.96	0.05	0.92
(1,40)	1:57:A:LYS:HB2	1:58:A:VAL:HG13	3	0.96	0.05	0.92
(1,40)	1:57:A:LYS:HB3	1:58:A:VAL:HG11	3	0.96	0.05	0.92
(1,40)	1:57:A:LYS:HB3	1:58:A:VAL:HG12	3	0.96	0.05	0.92
(1,40)	1:57:A:LYS:HB3	1:58:A:VAL:HG13	3	0.96	0.05	0.92
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD11	3	0.88	0.37	0.69
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD12	3	0.88	0.37	0.69
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD13	3	0.88	0.37	0.69
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD11	3	0.88	0.37	0.69
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD12	3	0.88	0.37	0.69

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD13	3	0.88	0.37	0.69
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD11	3	0.88	0.37	0.69
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD12	3	0.88	0.37	0.69
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD13	3	0.88	0.37	0.69
(1,195)	1:121:A:ARG:HG2	1:123:A:THR:H	3	0.84	0.47	0.95
(1,195)	1:121:A:ARG:HG3	1:123:A:THR:H	3	0.84	0.47	0.95
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD21	3	0.84	0.45	1.03
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD22	3	0.84	0.45	1.03
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD23	3	0.84	0.45	1.03
(1,3232)	1:32:A:ASP:HB3	1:27:A:LYS:H	3	0.8	0.34	0.72
(1,1116)	1:160:A:THR:HB	1:155:A:GLN:HA	3	0.78	0.56	0.72
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB1	3	0.77	0.68	0.46
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB2	3	0.77	0.68	0.46
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB3	3	0.77	0.68	0.46
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD11	3	0.77	0.21	0.84
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD12	3	0.77	0.21	0.84
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD13	3	0.77	0.21	0.84
(1,730)	1:22:A:TRP:HH2	1:26:A:LYS:HB2	3	0.75	0.85	0.18
(1,626)	1:177:A:THR:HB	1:170:A:ARG:H	3	0.74	0.33	0.6
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE1	3	0.67	0.25	0.74
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE2	3	0.67	0.25	0.74
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE3	3	0.67	0.25	0.74
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG21	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG22	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG23	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG21	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG22	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG23	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG21	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG22	3	0.66	0.33	0.66
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG23	3	0.66	0.33	0.66
(1,522)	1:96:A:GLU:HG2	1:93:A:ASN:H	3	0.66	0.31	0.46
(1,289)	1:149:A:ILE:HG21	2:201:A:Z90:HAI	3	0.66	0.37	0.56
(1,289)	1:149:A:ILE:HG22	2:201:A:Z90:HAI	3	0.66	0.37	0.56
(1,289)	1:149:A:ILE:HG23	2:201:A:Z90:HAI	3	0.66	0.37	0.56
(1,2198)	1:37:A:PHE:HD1	1:6:A:ASN:H	3	0.64	0.13	0.56
(1,2198)	1:37:A:PHE:HD2	1:6:A:ASN:H	3	0.64	0.13	0.56
(1,1953)	1:175:A:ASP:H	1:170:A:ARG:HG2	3	0.61	0.14	0.66
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD21	3	0.6	0.16	0.54
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD22	3	0.6	0.16	0.54
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD23	3	0.6	0.16	0.54
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD21	3	0.58	0.24	0.59

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD22	3	0.58	0.24	0.59
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD23	3	0.58	0.24	0.59
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD21	3	0.58	0.24	0.59
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD22	3	0.58	0.24	0.59
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD23	3	0.58	0.24	0.59
(1,2424)	1:96:A:GLU:HB3	1:93:A:ASN:H	3	0.58	0.05	0.56
(1,1271)	1:2:A:TYR:HD1	1:5:A:VAL:H	3	0.57	0.52	0.22
(1,1271)	1:2:A:TYR:HD2	1:5:A:VAL:H	3	0.57	0.52	0.22
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD1	3	0.56	0.04	0.56
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD2	3	0.56	0.04	0.56
(1,2192)	1:65:A:GLU:HG2	1:63:A:ALA:H	3	0.56	0.26	0.55
(1,2192)	1:65:A:GLU:HG3	1:63:A:ALA:H	3	0.56	0.26	0.55
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB2	3	0.55	0.1	0.58
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB3	3	0.55	0.1	0.58
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB1	3	0.55	0.48	0.31
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB2	3	0.55	0.48	0.31
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB3	3	0.55	0.48	0.31
(1,1026)	1:56:A:SER:HG	1:61:A:LEU:H	3	0.53	0.39	0.27
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG21	3	0.53	0.06	0.53
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG22	3	0.53	0.06	0.53
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG23	3	0.53	0.06	0.53
(1,2063)	1:93:A:ASN:HD22	1:93:A:ASN:H	3	0.53	0.05	0.5
(1,2092)	1:132:A:ILE:HD11	1:131:A:LEU:H	3	0.53	0.23	0.66
(1,2092)	1:132:A:ILE:HD12	1:131:A:LEU:H	3	0.53	0.23	0.66
(1,2092)	1:132:A:ILE:HD13	1:131:A:LEU:H	3	0.53	0.23	0.66
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG21	3	0.53	0.13	0.61
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG22	3	0.53	0.13	0.61
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG23	3	0.53	0.13	0.61
(1,3436)	1:34:A:GLU:H	1:35:A:GLY:H	3	0.53	0.06	0.56
(1,3108)	1:99:A:GLN:HE22	1:99:A:GLN:H	3	0.52	0.05	0.5
(1,49)	1:69:A:MET:HE1	1:61:A:LEU:HD21	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE1	1:61:A:LEU:HD22	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE1	1:61:A:LEU:HD23	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE2	1:61:A:LEU:HD21	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE2	1:61:A:LEU:HD22	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE2	1:61:A:LEU:HD23	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE3	1:61:A:LEU:HD21	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE3	1:61:A:LEU:HD22	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE3	1:61:A:LEU:HD23	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG21	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG22	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG23	3	0.5	0.11	0.56

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG21	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG22	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG23	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG21	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG22	3	0.5	0.11	0.56
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG23	3	0.5	0.11	0.56
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG21	3	0.5	0.01	0.5
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG22	3	0.5	0.01	0.5
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG23	3	0.5	0.01	0.5
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD2	3	0.49	0.08	0.44
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD3	3	0.49	0.08	0.44
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG11	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG12	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG13	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG11	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG12	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG13	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG11	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG12	3	0.49	0.45	0.21
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG13	3	0.49	0.45	0.21
(1,167)	1:174:A:CYS:H	1:170:A:ARG:HA	3	0.48	0.27	0.42
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD11	3	0.47	0.34	0.33
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD12	3	0.47	0.34	0.33
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD13	3	0.47	0.34	0.33
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	3	0.47	0.27	0.29
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	3	0.47	0.27	0.29
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	3	0.47	0.27	0.29
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG21	3	0.46	0.16	0.44
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG22	3	0.46	0.16	0.44
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG23	3	0.46	0.16	0.44
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD21	3	0.45	0.47	0.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD22	3	0.45	0.47	0.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD23	3	0.45	0.47	0.12
(1,3072)	1:165:A:LYS:HE2	1:165:A:LYS:H	3	0.43	0.08	0.47
(1,231)	1:145:A:ILE:HG21	1:144:A:ASP:H	3	0.42	0.04	0.42
(1,231)	1:145:A:ILE:HG22	1:144:A:ASP:H	3	0.42	0.04	0.42
(1,231)	1:145:A:ILE:HG23	1:144:A:ASP:H	3	0.42	0.04	0.42
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE1	3	0.42	0.25	0.27
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE2	3	0.42	0.25	0.27
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE3	3	0.42	0.25	0.27
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG11	3	0.41	0.23	0.46
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG12	3	0.41	0.23	0.46

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG13	3	0.41	0.23	0.46
(1,313)	1:39:A:VAL:HG21	2:201:A:Z90:HAE	3	0.41	0.2	0.54
(1,313)	1:39:A:VAL:HG22	2:201:A:Z90:HAE	3	0.41	0.2	0.54
(1,313)	1:39:A:VAL:HG23	2:201:A:Z90:HAE	3	0.41	0.2	0.54
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB1	3	0.41	0.22	0.44
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB2	3	0.41	0.22	0.44
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB3	3	0.41	0.22	0.44
(1,1480)	1:171:A:ASN:HD22	1:171:A:ASN:HA	3	0.41	0.12	0.34
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG12	3	0.41	0.24	0.25
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG13	3	0.41	0.24	0.25
(1,2819)	1:160:A:THR:HB	1:159:A:GLY:H	3	0.41	0.22	0.34
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB2	3	0.4	0.15	0.46
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB3	3	0.4	0.15	0.46
(1,2672)	1:179:A:PHE:HE1	1:146:A:VAL:H	3	0.4	0.15	0.33
(1,2672)	1:179:A:PHE:HE2	1:146:A:VAL:H	3	0.4	0.15	0.33
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG21	3	0.38	0.24	0.34
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG22	3	0.38	0.24	0.34
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG23	3	0.38	0.24	0.34
(1,2781)	1:9:A:LEU:HD21	1:13:A:VAL:H	3	0.38	0.33	0.18
(1,2781)	1:9:A:LEU:HD22	1:13:A:VAL:H	3	0.38	0.33	0.18
(1,2781)	1:9:A:LEU:HD23	1:13:A:VAL:H	3	0.38	0.33	0.18
(1,564)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	3	0.36	0.1	0.33
(1,810)	1:57:A:LYS:HG3	1:55:A:ALA:H	3	0.33	0.1	0.27
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG21	3	0.33	0.14	0.4
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG22	3	0.33	0.14	0.4
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG23	3	0.33	0.14	0.4
(1,2660)	1:184:A:LYS:HE3	1:184:A:LYS:H	3	0.33	0.07	0.34
(1,853)	1:171:A:ASN:HD22	1:173:A:GLU:H	3	0.32	0.11	0.37
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD1	3	0.31	0.23	0.17
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD2	3	0.31	0.23	0.17
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD11	3	0.31	0.01	0.31
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD12	3	0.31	0.01	0.31
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD13	3	0.31	0.01	0.31
(1,1469)	1:171:A:ASN:HD22	1:171:A:ASN:HA	3	0.3	0.12	0.24
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB1	3	0.3	0.08	0.33
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB2	3	0.3	0.08	0.33
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB3	3	0.3	0.08	0.33
(1,2159)	1:131:A:LEU:HA	1:126:A:GLU:H	3	0.29	0.13	0.34
(1,3466)	1:93:A:ASN:HA	1:96:A:GLU:H	3	0.29	0.09	0.27
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD11	3	0.29	0.23	0.14
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD12	3	0.29	0.23	0.14
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD13	3	0.29	0.23	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,266)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	3	0.28	0.08	0.28
(1,266)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	3	0.28	0.08	0.28
(1,266)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	3	0.28	0.08	0.28
(1,188)	1:165:A:LYS:HD2	1:166:A:VAL:H	3	0.28	0.05	0.26
(1,188)	1:165:A:LYS:HD3	1:166:A:VAL:H	3	0.28	0.05	0.26
(1,3012)	1:176:A:HIS:H	1:174:A:CYS:HB3	3	0.28	0.16	0.25
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD11	3	0.28	0.01	0.28
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD12	3	0.28	0.01	0.28
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD13	3	0.28	0.01	0.28
(1,3443)	1:143:A:GLN:HG3	1:144:A:ASP:H	3	0.27	0.03	0.28
(1,114)	1:182:A:GLU:H	1:164:A:MET:H	3	0.25	0.07	0.3
(1,114)	1:165:A:LYS:H	1:182:A:GLU:H	3	0.25	0.07	0.3
(1,135)	1:59:A:LEU:HA	1:61:A:LEU:H	3	0.25	0.04	0.23
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD11	3	0.25	0.02	0.26
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD12	3	0.25	0.02	0.26
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD13	3	0.25	0.02	0.26
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG11	3	0.25	0.04	0.27
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG12	3	0.25	0.04	0.27
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG13	3	0.25	0.04	0.27
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD11	3	0.25	0.11	0.24
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD12	3	0.25	0.11	0.24
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD13	3	0.25	0.11	0.24
(1,2734)	1:14:A:ILE:HB	1:16:A:ASN:H	3	0.24	0.07	0.24
(1,268)	1:101:A:LEU:HD21	2:201:A:Z90:HAI	3	0.23	0.12	0.17
(1,268)	1:101:A:LEU:HD22	2:201:A:Z90:HAI	3	0.23	0.12	0.17
(1,268)	1:101:A:LEU:HD23	2:201:A:Z90:HAI	3	0.23	0.12	0.17
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG11	3	0.23	0.03	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG12	3	0.23	0.03	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG13	3	0.23	0.03	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG21	3	0.23	0.03	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG22	3	0.23	0.03	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG23	3	0.23	0.03	0.22
(1,535)	1:129:A:LYS:HA	1:131:A:LEU:H	3	0.23	0.06	0.26
(1,2560)	1:141:A:GLY:HA3	1:144:A:ASP:H	3	0.23	0.06	0.26
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD21	3	0.23	0.06	0.19
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD22	3	0.23	0.06	0.19
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD23	3	0.23	0.06	0.19
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG21	3	0.22	0.03	0.23
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG22	3	0.22	0.03	0.23
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG23	3	0.22	0.03	0.23
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG21	3	0.22	0.03	0.23
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG22	3	0.22	0.03	0.23

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG23	3	0.22	0.03	0.23
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG21	3	0.22	0.03	0.23
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG22	3	0.22	0.03	0.23
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG23	3	0.22	0.03	0.23
(1,9)	1:127:A:LYS:HA	1:128:A:GLY:HA2	3	0.22	0.05	0.23
(1,9)	1:127:A:LYS:HA	1:126:A:GLU:HA	3	0.22	0.05	0.23
(1,298)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	3	0.21	0.05	0.21
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD21	3	0.21	0.04	0.23
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD22	3	0.21	0.04	0.23
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD23	3	0.21	0.04	0.23
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD11	3	0.21	0.0	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD12	3	0.21	0.0	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD13	3	0.21	0.0	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD21	3	0.21	0.0	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD22	3	0.21	0.0	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD23	3	0.21	0.0	0.21
(1,2680)	1:180:A:LEU:HA	1:167:A:ILE:H	3	0.21	0.08	0.17
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD2	3	0.21	0.04	0.22
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD3	3	0.21	0.04	0.22
(1,1179)	1:167:A:ILE:HG12	1:179:A:PHE:H	3	0.2	0.07	0.22
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE1	3	0.2	0.07	0.21
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE2	3	0.2	0.07	0.21
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE1	3	0.2	0.04	0.21
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE2	3	0.2	0.04	0.21
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE3	3	0.2	0.04	0.21
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG11	3	0.2	0.06	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG12	3	0.2	0.06	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG13	3	0.2	0.06	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG21	3	0.2	0.06	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG22	3	0.2	0.06	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG23	3	0.2	0.06	0.18
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD11	3	0.2	0.01	0.2
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD12	3	0.2	0.01	0.2
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD13	3	0.2	0.01	0.2
(1,444)	1:131:A:LEU:HG	1:132:A:ILE:H	3	0.19	0.03	0.19
(1,381)	1:100:A:ASN:H	1:99:A:GLN:H	3	0.19	0.04	0.17
(1,1693)	1:48:A:THR:HG1	1:48:A:THR:H	3	0.19	0.05	0.19
(1,2675)	1:60:A:ASN:HD22	1:60:A:ASN:HB2	3	0.19	0.02	0.18
(1,2423)	1:183:A:GLU:HB3	1:184:A:LYS:H	3	0.18	0.08	0.15
(1,761)	1:159:A:GLY:HA3	1:158:A:HIS:H	3	0.18	0.05	0.2
(1,1035)	1:170:A:ARG:HE	1:170:A:ARG:HG3	3	0.15	0.04	0.17
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG21	3	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG22	3	0.15	0.03	0.16
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG23	3	0.15	0.03	0.16
(1,1409)	1:14:A:ILE:HB	1:18:A:GLY:H	3	0.15	0.03	0.17
(1,1169)	1:17:A:TYR:HE1	1:16:A:ASN:H	3	0.15	0.01	0.15
(1,1169)	1:17:A:TYR:HE2	1:16:A:ASN:H	3	0.15	0.01	0.15
(1,3207)	1:35:A:GLY:HA3	1:36:A:GLN:H	3	0.15	0.01	0.15
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB1	3	0.14	0.03	0.14
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB2	3	0.14	0.03	0.14
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB3	3	0.14	0.03	0.14
(1,219)	1:56:A:SER:H	1:53:A:ALA:HB1	3	0.14	0.03	0.14
(1,219)	1:56:A:SER:H	1:53:A:ALA:HB2	3	0.14	0.03	0.14
(1,219)	1:56:A:SER:H	1:53:A:ALA:HB3	3	0.14	0.03	0.14
(1,2296)	1:37:A:PHE:HA	1:38:A:LEU:H	3	0.14	0.02	0.13
(1,3001)	1:137:A:SER:H	1:136:A:TYR:HB2	3	0.13	0.02	0.12
(1,1456)	1:160:A:THR:HB	1:158:A:HIS:H	2	1.88	0.36	1.88
(1,2289)	1:158:A:HIS:HB3	1:160:A:THR:H	2	1.72	0.32	1.72
(1,3463)	1:170:A:ARG:HE	1:176:A:HIS:H	2	1.63	0.11	1.63
(1,2204)	1:56:A:SER:HB2	1:55:A:ALA:H	2	1.27	0.06	1.27
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG11	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG12	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG13	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG11	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG12	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG13	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG11	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG12	2	1.24	0.12	1.24
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG13	2	1.24	0.12	1.24
(1,909)	1:65:A:GLU:HG2	1:64:A:GLY:H	2	1.21	0.02	1.21
(1,909)	1:65:A:GLU:HG3	1:64:A:GLY:H	2	1.21	0.02	1.21
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG21	2	1.14	0.32	1.14
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG22	2	1.14	0.32	1.14
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG23	2	1.14	0.32	1.14
(1,994)	1:165:A:LYS:HE3	1:180:A:LEU:H	2	1.14	0.31	1.14
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE1	2	1.13	0.44	1.13
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE2	2	1.13	0.44	1.13
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE3	2	1.13	0.44	1.13
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	2	1.12	0.12	1.12
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	2	1.12	0.12	1.12
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	2	1.12	0.12	1.12
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD21	2	1.09	0.82	1.09
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD22	2	1.09	0.82	1.09
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD23	2	1.09	0.82	1.09

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD21	2	1.09	0.82	1.09
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD22	2	1.09	0.82	1.09
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD23	2	1.09	0.82	1.09
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD21	2	1.09	0.82	1.09
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD22	2	1.09	0.82	1.09
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD23	2	1.09	0.82	1.09
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG11	2	1.07	0.42	1.07
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG12	2	1.07	0.42	1.07
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG13	2	1.07	0.42	1.07
(1,2237)	1:120:A:PHE:HA	1:135:A:TYR:H	2	1.06	0.84	1.06
(1,3457)	1:188:A:GLU:H	1:186:A:SER:HA	2	1.05	0.25	1.05
(1,1415)	1:34:A:GLU:HA	1:36:A:GLN:H	2	1.02	0.6	1.02
(1,3435)	1:146:A:VAL:HB	1:144:A:ASP:H	2	1.01	0.32	1.01
(1,338)	1:139:A:ARG:HG2	1:49:A:TYR:HE1	2	1.01	0.58	1.01
(1,338)	1:139:A:ARG:HG2	1:49:A:TYR:HE2	2	1.01	0.58	1.01
(1,2212)	1:184:A:LYS:HD2	1:184:A:LYS:H	2	1.0	0.26	1.0
(1,2212)	1:184:A:LYS:HD3	1:184:A:LYS:H	2	1.0	0.26	1.0
(1,3563)	1:131:A:LEU:HB3	1:181:A:ILE:H	2	1.0	0.19	1.0
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG11	2	0.98	0.01	0.98
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG12	2	0.98	0.01	0.98
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG13	2	0.98	0.01	0.98
(1,1930)	1:158:A:HIS:HB2	1:160:A:THR:H	2	0.94	0.5	0.94
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD11	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD12	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD13	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD21	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD22	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD23	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD11	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD12	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD13	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD21	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD22	2	0.93	0.73	0.93
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD23	2	0.93	0.73	0.93
(1,2896)	1:136:A:TYR:H	1:119:A:SER:H	2	0.9	0.05	0.9
(1,1752)	1:43:A:TYR:HE1	1:37:A:PHE:HE1	2	0.89	0.47	0.89
(1,1752)	1:43:A:TYR:HE1	1:37:A:PHE:HE2	2	0.89	0.47	0.89
(1,1752)	1:43:A:TYR:HE2	1:37:A:PHE:HE1	2	0.89	0.47	0.89
(1,1752)	1:43:A:TYR:HE2	1:37:A:PHE:HE2	2	0.89	0.47	0.89
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	2	0.88	0.47	0.88
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	2	0.88	0.47	0.88
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	2	0.88	0.47	0.88

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	2	0.88	0.47	0.88
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	2	0.88	0.47	0.88
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	2	0.88	0.47	0.88
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	2	0.88	0.47	0.88
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	2	0.88	0.47	0.88
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	2	0.88	0.47	0.88
(1,2565)	1:135:A:TYR:HB2	1:179:A:PHE:H	2	0.88	0.56	0.88
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD21	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD22	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD23	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD21	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD22	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD23	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD21	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD22	2	0.88	0.5	0.88
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD23	2	0.88	0.5	0.88
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD11	2	0.86	0.72	0.86
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD12	2	0.86	0.72	0.86
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD13	2	0.86	0.72	0.86
(1,1530)	1:126:A:GLU:HG3	1:127:A:LYS:H	2	0.84	0.67	0.84
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD11	2	0.79	0.05	0.79
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD12	2	0.79	0.05	0.79
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD13	2	0.79	0.05	0.79
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD11	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD12	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD13	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD11	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD12	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD13	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD11	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD12	2	0.77	0.05	0.77
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD13	2	0.77	0.05	0.77
(1,1825)	1:96:A:GLU:HG3	1:93:A:ASN:H	2	0.76	0.05	0.76
(1,1539)	1:1:A:MET:HE1	1:5:A:VAL:HB	2	0.75	0.63	0.75
(1,1539)	1:1:A:MET:HE2	1:5:A:VAL:HB	2	0.75	0.63	0.75
(1,1539)	1:1:A:MET:HE3	1:5:A:VAL:HB	2	0.75	0.63	0.75
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG21	2	0.73	0.05	0.73
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG22	2	0.73	0.05	0.73
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG23	2	0.73	0.05	0.73
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD11	2	0.72	0.03	0.72
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD12	2	0.72	0.03	0.72
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD13	2	0.72	0.03	0.72

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG21	2	0.72	0.38	0.72
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG22	2	0.72	0.38	0.72
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG23	2	0.72	0.38	0.72
(1,96)	1:180:A:LEU:HG	1:131:A:LEU:H	2	0.71	0.56	0.71
(1,2967)	1:160:A:THR:H	1:157:A:ILE:H	2	0.7	0.5	0.7
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG11	2	0.66	0.01	0.66
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG12	2	0.66	0.01	0.66
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG13	2	0.66	0.01	0.66
(1,2743)	1:62:A:ASN:HD22	1:65:A:GLU:HB2	2	0.66	0.16	0.66
(1,2743)	1:62:A:ASN:HD22	1:65:A:GLU:HB3	2	0.66	0.16	0.66
(1,1172)	1:135:A:TYR:HD1	1:177:A:THR:H	2	0.64	0.12	0.64
(1,1172)	1:135:A:TYR:HD2	1:177:A:THR:H	2	0.64	0.12	0.64
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD21	2	0.63	0.11	0.63
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD22	2	0.63	0.11	0.63
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD23	2	0.63	0.11	0.63
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD21	2	0.63	0.11	0.63
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD22	2	0.63	0.11	0.63
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD23	2	0.63	0.11	0.63
(1,2805)	1:26:A:LYS:HE3	1:22:A:TRP:HE1	2	0.62	0.38	0.62
(1,318)	1:101:A:LEU:HD21	2:201:A:Z90:HAM	2	0.62	0.05	0.62
(1,318)	1:101:A:LEU:HD22	2:201:A:Z90:HAM	2	0.62	0.05	0.62
(1,318)	1:101:A:LEU:HD23	2:201:A:Z90:HAM	2	0.62	0.05	0.62
(1,2025)	1:47:A:LYS:HE2	1:47:A:LYS:H	2	0.62	0.07	0.62
(1,264)	1:101:A:LEU:HD21	2:201:A:Z90:HAM	2	0.6	0.04	0.6
(1,264)	1:101:A:LEU:HD22	2:201:A:Z90:HAM	2	0.6	0.04	0.6
(1,264)	1:101:A:LEU:HD23	2:201:A:Z90:HAM	2	0.6	0.04	0.6
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD21	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD22	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD23	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD21	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD22	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD23	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD21	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD22	2	0.6	0.22	0.6
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD23	2	0.6	0.22	0.6
(1,1876)	1:10:A:GLU:HG3	1:22:A:TRP:HE1	2	0.59	0.43	0.59
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG21	2	0.58	0.1	0.58
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG22	2	0.58	0.1	0.58
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG23	2	0.58	0.1	0.58
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG21	2	0.58	0.1	0.58
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG22	2	0.58	0.1	0.58
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG23	2	0.58	0.1	0.58

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1820)	1:56:A:SER:HG	1:62:A:ASN:H	2	0.57	0.09	0.57
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD11	2	0.56	0.23	0.56
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD12	2	0.56	0.23	0.56
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD13	2	0.56	0.23	0.56
(1,479)	1:42:A:ILE:HA	1:3:A:GLY:H	2	0.55	0.05	0.55
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG11	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG12	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG13	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG11	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG12	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG13	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG11	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG12	2	0.55	0.39	0.55
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG13	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD11	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD12	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD13	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD11	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD12	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD13	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD11	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD12	2	0.55	0.39	0.55
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD13	2	0.55	0.39	0.55
(1,1864)	1:38:A:LEU:HB2	1:41:A:ILE:H	2	0.54	0.38	0.54
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE1	2	0.54	0.07	0.54
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE2	2	0.54	0.07	0.54
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE3	2	0.54	0.07	0.54
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG21	2	0.52	0.11	0.52
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG22	2	0.52	0.11	0.52
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG23	2	0.52	0.11	0.52
(1,277)	1:149:A:ILE:HG21	2:201:A:Z90:HAM	2	0.52	0.04	0.52
(1,277)	1:149:A:ILE:HG22	2:201:A:Z90:HAM	2	0.52	0.04	0.52
(1,277)	1:149:A:ILE:HG23	2:201:A:Z90:HAM	2	0.52	0.04	0.52
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD11	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD12	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD13	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD11	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD12	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD13	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD11	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD12	2	0.52	0.22	0.52
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD13	2	0.52	0.22	0.52

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG21	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG22	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG23	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG21	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG22	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG23	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG21	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG22	2	0.52	0.0	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG23	2	0.52	0.0	0.52
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD11	2	0.52	0.04	0.52
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD12	2	0.52	0.04	0.52
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD13	2	0.52	0.04	0.52
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD11	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD12	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD13	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD11	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD12	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD13	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD11	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD12	2	0.5	0.24	0.5
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD13	2	0.5	0.24	0.5
(1,3185)	1:16:A:ASN:HD22	1:16:A:ASN:H	2	0.5	0.08	0.5
(1,189)	1:2:A:TYR:HD1	1:6:A:ASN:H	2	0.49	0.23	0.49
(1,189)	1:2:A:TYR:HD2	1:6:A:ASN:H	2	0.49	0.23	0.49
(1,189)	1:43:A:TYR:HD1	1:6:A:ASN:H	2	0.49	0.23	0.49
(1,189)	1:43:A:TYR:HD2	1:6:A:ASN:H	2	0.49	0.23	0.49
(1,305)	1:149:A:ILE:HG21	2:201:A:Z90:HAM	2	0.49	0.04	0.49
(1,305)	1:149:A:ILE:HG22	2:201:A:Z90:HAM	2	0.49	0.04	0.49
(1,305)	1:149:A:ILE:HG23	2:201:A:Z90:HAM	2	0.49	0.04	0.49
(1,1533)	1:161:A:GLU:HA	1:184:A:LYS:H	2	0.49	0.15	0.49
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG21	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG22	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG23	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG21	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG22	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG23	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG21	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG22	2	0.49	0.16	0.49
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG23	2	0.49	0.16	0.49
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG21	2	0.49	0.32	0.49
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG22	2	0.49	0.32	0.49
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG23	2	0.49	0.32	0.49

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG21	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG22	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG23	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG21	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG22	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG23	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG21	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG22	2	0.46	0.01	0.46
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG23	2	0.46	0.01	0.46
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD11	2	0.46	0.21	0.46
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD12	2	0.46	0.21	0.46
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD13	2	0.46	0.21	0.46
(1,2798)	1:10:A:GLU:HA	1:22:A:TRP:HE1	2	0.46	0.34	0.46
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG21	2	0.44	0.02	0.44
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG22	2	0.44	0.02	0.44
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG23	2	0.44	0.02	0.44
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG21	2	0.44	0.02	0.44
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG22	2	0.44	0.02	0.44
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG23	2	0.44	0.02	0.44
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB1	2	0.44	0.01	0.44
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB2	2	0.44	0.01	0.44
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB3	2	0.44	0.01	0.44
(1,1404)	1:50:A:ASP:HB3	1:49:A:TYR:H	2	0.44	0.32	0.44
(1,198)	1:120:A:PHE:HA	1:135:A:TYR:H	2	0.42	0.2	0.42
(1,198)	1:135:A:TYR:HE1	1:135:A:TYR:H	2	0.42	0.2	0.42
(1,198)	1:135:A:TYR:HE2	1:135:A:TYR:H	2	0.42	0.2	0.42
(1,1038)	1:177:A:THR:HA	1:169:A:GLN:H	2	0.42	0.08	0.42
(1,3233)	1:141:A:GLY:HA2	1:140:A:GLU:H	2	0.42	0.08	0.42
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE1	2	0.42	0.2	0.42
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE2	2	0.42	0.2	0.42
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE3	2	0.42	0.2	0.42
(1,2421)	1:72:A:LYS:H	1:148:A:GLY:H	2	0.42	0.05	0.42
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD11	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD12	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD13	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD11	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD12	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD13	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD11	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD12	2	0.41	0.01	0.41
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD13	2	0.41	0.01	0.41
(1,2841)	1:65:A:GLU:HG2	1:65:A:GLU:H	2	0.41	0.04	0.41

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2841)	1:65:A:GLU:HG3	1:65:A:GLU:H	2	0.41	0.04	0.41
(1,183)	1:3:A:GLY:H	1:43:A:TYR:HE1	2	0.4	0.1	0.4
(1,183)	1:3:A:GLY:H	1:43:A:TYR:HE2	2	0.4	0.1	0.4
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG21	2	0.38	0.06	0.38
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG22	2	0.38	0.06	0.38
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG23	2	0.38	0.06	0.38
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG11	2	0.38	0.2	0.38
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG12	2	0.38	0.2	0.38
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG13	2	0.38	0.2	0.38
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG21	2	0.36	0.04	0.36
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG22	2	0.36	0.04	0.36
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG23	2	0.36	0.04	0.36
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG21	2	0.36	0.01	0.36
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG22	2	0.36	0.01	0.36
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG23	2	0.36	0.01	0.36
(1,2700)	1:120:A:PHE:HA	1:134:A:HIS:H	2	0.35	0.15	0.35
(1,1447)	1:146:A:VAL:HB	1:148:A:GLY:H	2	0.34	0.08	0.34
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD11	2	0.34	0.16	0.34
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD12	2	0.34	0.16	0.34
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD13	2	0.34	0.16	0.34
(1,794)	1:136:A:TYR:HD1	1:177:A:THR:H	2	0.34	0.2	0.34
(1,794)	1:136:A:TYR:HD2	1:177:A:THR:H	2	0.34	0.2	0.34
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD11	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD12	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD13	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD11	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD12	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD13	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD11	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD12	2	0.34	0.14	0.34
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD13	2	0.34	0.14	0.34
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD21	2	0.32	0.0	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD22	2	0.32	0.0	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD23	2	0.32	0.0	0.32
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD11	2	0.32	0.02	0.32
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD12	2	0.32	0.02	0.32
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD13	2	0.32	0.02	0.32
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG11	2	0.31	0.03	0.31
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG12	2	0.31	0.03	0.31
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG13	2	0.31	0.03	0.31
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG21	2	0.31	0.03	0.31
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG22	2	0.31	0.03	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG23	2	0.31	0.03	0.31
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD21	2	0.31	0.04	0.31
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD22	2	0.31	0.04	0.31
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD23	2	0.31	0.04	0.31
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD21	2	0.31	0.04	0.31
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD22	2	0.31	0.04	0.31
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD23	2	0.31	0.04	0.31
(1,2412)	1:24:A:ASP:HB3	1:23:A:GLU:H	2	0.31	0.01	0.31
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD11	2	0.3	0.16	0.3
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD12	2	0.3	0.16	0.3
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD13	2	0.3	0.16	0.3
(1,1968)	1:3:A:GLY:H	1:43:A:TYR:HE1	2	0.3	0.0	0.3
(1,1968)	1:3:A:GLY:H	1:43:A:TYR:HE2	2	0.3	0.0	0.3
(1,2780)	1:26:A:LYS:HG3	1:22:A:TRP:HE1	2	0.3	0.11	0.3
(1,823)	1:183:A:GLU:HA	1:162:A:ILE:H	2	0.3	0.01	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD11	2	0.3	0.01	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD12	2	0.3	0.01	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD13	2	0.3	0.01	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD21	2	0.3	0.01	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD22	2	0.3	0.01	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD23	2	0.3	0.01	0.3
(1,2467)	1:125:A:ALA:H	1:130:A:GLY:H	2	0.29	0.16	0.29
(1,3039)	1:32:A:ASP:HB3	1:27:A:LYS:HA	2	0.29	0.1	0.29
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB1	2	0.28	0.11	0.28
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB2	2	0.28	0.11	0.28
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB3	2	0.28	0.11	0.28
(1,566)	1:61:A:LEU:H	1:57:A:LYS:H	2	0.28	0.15	0.28
(1,1890)	1:120:A:PHE:H	1:120:A:PHE:HD1	2	0.28	0.15	0.28
(1,1890)	1:120:A:PHE:H	1:120:A:PHE:HD2	2	0.28	0.15	0.28
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB1	2	0.28	0.14	0.28
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB2	2	0.28	0.14	0.28
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB3	2	0.28	0.14	0.28
(1,2019)	1:83:A:TYR:H	1:83:A:TYR:HD1	2	0.28	0.08	0.28
(1,2019)	1:83:A:TYR:H	1:83:A:TYR:HD2	2	0.28	0.08	0.28
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD21	2	0.28	0.13	0.28
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD22	2	0.28	0.13	0.28
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD23	2	0.28	0.13	0.28
(1,3308)	1:27:A:LYS:HG3	1:28:A:GLU:H	2	0.28	0.06	0.28
(1,1472)	1:104:A:LEU:HD21	2:201:A:Z90:HAP	2	0.27	0.08	0.27
(1,1472)	1:104:A:LEU:HD22	2:201:A:Z90:HAP	2	0.27	0.08	0.27
(1,1472)	1:104:A:LEU:HD23	2:201:A:Z90:HAP	2	0.27	0.08	0.27
(1,3043)	1:57:A:LYS:H	1:25:A:ILE:HG12	2	0.27	0.02	0.27

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3043)	1:57:A:LYS:H	1:25:A:ILE:HG13	2	0.27	0.02	0.27
(1,3137)	1:19:A:PRO:HD3	1:22:A:TRP:H	2	0.27	0.12	0.27
(1,3358)	1:75:A:PHE:HE1	1:157:A:ILE:H	2	0.27	0.15	0.27
(1,3358)	1:75:A:PHE:HE2	1:157:A:ILE:H	2	0.27	0.15	0.27
(1,1372)	1:124:A:ASP:HB2	1:125:A:ALA:H	2	0.26	0.01	0.26
(1,3149)	1:93:A:ASN:HA	1:95:A:ARG:H	2	0.26	0.04	0.26
(1,501)	1:126:A:GLU:HG3	1:126:A:GLU:H	2	0.26	0.12	0.26
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD11	2	0.25	0.01	0.25
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD12	2	0.25	0.01	0.25
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD13	2	0.25	0.01	0.25
(1,1672)	1:173:A:GLU:HG3	1:174:A:CYS:H	2	0.24	0.1	0.24
(1,160)	1:171:A:ASN:H	1:174:A:CYS:HB2	2	0.24	0.05	0.24
(1,160)	1:171:A:ASN:H	1:174:A:CYS:HB3	2	0.24	0.05	0.24
(1,2002)	1:174:A:CYS:H	1:173:A:GLU:HB3	2	0.24	0.02	0.24
(1,2640)	1:61:A:LEU:H	1:59:A:LEU:HG	2	0.24	0.02	0.24
(1,1335)	1:170:A:ARG:H	1:178:A:GLN:H	2	0.24	0.05	0.24
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD11	2	0.24	0.04	0.24
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD12	2	0.24	0.04	0.24
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD13	2	0.24	0.04	0.24
(1,3408)	1:140:A:GLU:HB3	1:169:A:GLN:HE22	2	0.24	0.05	0.24
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG21	2	0.24	0.05	0.24
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG22	2	0.24	0.05	0.24
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG23	2	0.24	0.05	0.24
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG21	2	0.24	0.05	0.24
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG22	2	0.24	0.05	0.24
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG23	2	0.24	0.05	0.24
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD21	2	0.23	0.08	0.23
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD22	2	0.23	0.08	0.23
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD23	2	0.23	0.08	0.23
(1,3506)	1:176:A:HIS:H	1:170:A:ARG:HG3	2	0.23	0.01	0.23
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD11	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD12	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD13	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD11	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD12	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD13	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD11	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD12	2	0.23	0.06	0.23
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD13	2	0.23	0.06	0.23
(1,3447)	1:66:A:ILE:HB	1:63:A:ALA:H	2	0.22	0.05	0.22
(1,3549)	1:165:A:LYS:HG2	1:180:A:LEU:H	2	0.22	0.08	0.22
(1,1274)	1:5:A:VAL:HG11	1:5:A:VAL:H	2	0.22	0.09	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1274)	1:5:A:VAL:HG12	1:5:A:VAL:H	2	0.22	0.09	0.22
(1,1274)	1:5:A:VAL:HG13	1:5:A:VAL:H	2	0.22	0.09	0.22
(1,2384)	1:115:A:MET:HE1	1:115:A:MET:HB3	2	0.22	0.02	0.22
(1,2384)	1:115:A:MET:HE2	1:115:A:MET:HB3	2	0.22	0.02	0.22
(1,2384)	1:115:A:MET:HE3	1:115:A:MET:HB3	2	0.22	0.02	0.22
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD11	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD12	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD13	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD11	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD12	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD13	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD11	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD12	2	0.22	0.08	0.22
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD13	2	0.22	0.08	0.22
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG21	2	0.22	0.04	0.22
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG22	2	0.22	0.04	0.22
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG23	2	0.22	0.04	0.22
(1,3455)	1:95:A:ARG:HD2	1:96:A:GLU:H	2	0.22	0.06	0.22
(1,3455)	1:95:A:ARG:HD3	1:96:A:GLU:H	2	0.22	0.06	0.22
(1,2015)	1:47:A:LYS:HE3	1:47:A:LYS:HA	2	0.22	0.01	0.22
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD11	2	0.22	0.1	0.22
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD12	2	0.22	0.1	0.22
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD13	2	0.22	0.1	0.22
(1,69)	1:142:A:LEU:HD11	1:48:A:THR:HG21	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD11	1:48:A:THR:HG22	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD11	1:48:A:THR:HG23	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD12	1:48:A:THR:HG21	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD12	1:48:A:THR:HG22	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD12	1:48:A:THR:HG23	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD13	1:48:A:THR:HG21	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD13	1:48:A:THR:HG22	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD13	1:48:A:THR:HG23	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD11	1:67:A:LEU:HD21	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD11	1:67:A:LEU:HD22	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD11	1:67:A:LEU:HD23	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD12	1:67:A:LEU:HD21	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD12	1:67:A:LEU:HD22	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD12	1:67:A:LEU:HD23	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD13	1:67:A:LEU:HD21	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD13	1:67:A:LEU:HD22	2	0.21	0.04	0.21
(1,69)	1:142:A:LEU:HD13	1:67:A:LEU:HD23	2	0.21	0.04	0.21
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG21	2	0.21	0.06	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG22	2	0.21	0.06	0.21
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG23	2	0.21	0.06	0.21
(1,1842)	1:184:A:LYS:HA	1:184:A:LYS:HD2	2	0.21	0.03	0.21
(1,1842)	1:184:A:LYS:HA	1:184:A:LYS:HD3	2	0.21	0.03	0.21
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG11	2	0.21	0.08	0.21
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG12	2	0.21	0.08	0.21
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG13	2	0.21	0.08	0.21
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD11	2	0.2	0.04	0.2
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD12	2	0.2	0.04	0.2
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD13	2	0.2	0.04	0.2
(1,3584)	1:168:A:GLN:H	1:180:A:LEU:H	2	0.2	0.03	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD11	2	0.2	0.0	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD12	2	0.2	0.0	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD13	2	0.2	0.0	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD11	2	0.2	0.0	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD12	2	0.2	0.0	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD13	2	0.2	0.0	0.2
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD11	2	0.2	0.03	0.2
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD12	2	0.2	0.03	0.2
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD13	2	0.2	0.03	0.2
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB1	2	0.2	0.09	0.2
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB2	2	0.2	0.09	0.2
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB3	2	0.2	0.09	0.2
(1,2226)	1:161:A:GLU:HG3	1:161:A:GLU:H	2	0.2	0.02	0.2
(1,181)	1:40:A:ARG:HG2	1:40:A:ARG:H	2	0.19	0.05	0.19
(1,181)	1:40:A:ARG:HG3	1:40:A:ARG:H	2	0.19	0.05	0.19
(1,1949)	1:175:A:ASP:H	1:170:A:ARG:HG3	2	0.19	0.03	0.19
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD11	2	0.18	0.01	0.18
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD12	2	0.18	0.01	0.18
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD13	2	0.18	0.01	0.18
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	2	0.18	0.03	0.18
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	2	0.18	0.03	0.18
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	2	0.18	0.03	0.18
(1,697)	1:127:A:LYS:HA	1:128:A:GLY:HA3	2	0.18	0.02	0.18
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG21	2	0.18	0.02	0.18
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG22	2	0.18	0.02	0.18
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG23	2	0.18	0.02	0.18
(1,1262)	1:176:A:HIS:H	1:170:A:ARG:HB2	2	0.18	0.0	0.18
(1,1262)	1:176:A:HIS:H	1:170:A:ARG:HB3	2	0.18	0.0	0.18
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB1	2	0.18	0.07	0.18
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB2	2	0.18	0.07	0.18
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB3	2	0.18	0.07	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2101)	1:140:A:GLU:HB3	1:169:A:GLN:HE22	2	0.18	0.04	0.18
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB1	2	0.18	0.0	0.18
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB2	2	0.18	0.0	0.18
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB3	2	0.18	0.0	0.18
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG21	2	0.18	0.02	0.18
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG22	2	0.18	0.02	0.18
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG23	2	0.18	0.02	0.18
(1,2712)	1:83:A:TYR:H	1:82:A:GLY:HA2	2	0.18	0.06	0.18
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD21	2	0.16	0.06	0.16
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD22	2	0.16	0.06	0.16
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD23	2	0.16	0.06	0.16
(1,90)	1:27:A:LYS:HE2	1:27:A:LYS:H	2	0.16	0.02	0.16
(1,90)	1:27:A:LYS:HE3	1:27:A:LYS:H	2	0.16	0.02	0.16
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD11	2	0.16	0.03	0.16
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD12	2	0.16	0.03	0.16
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD13	2	0.16	0.03	0.16
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD11	2	0.16	0.03	0.16
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD12	2	0.16	0.03	0.16
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD13	2	0.16	0.03	0.16
(1,2886)	1:134:A:HIS:HD2	1:134:A:HIS:H	2	0.16	0.04	0.16
(1,271)	1:150:A:ILE:HD11	2:201:A:Z90:HAI	2	0.15	0.02	0.15
(1,271)	1:150:A:ILE:HD12	2:201:A:Z90:HAI	2	0.15	0.02	0.15
(1,271)	1:150:A:ILE:HD13	2:201:A:Z90:HAI	2	0.15	0.02	0.15
(1,2676)	1:153:A:VAL:HG21	1:153:A:VAL:H	2	0.15	0.01	0.15
(1,2676)	1:153:A:VAL:HG22	1:153:A:VAL:H	2	0.15	0.01	0.15
(1,2676)	1:153:A:VAL:HG23	1:153:A:VAL:H	2	0.15	0.01	0.15
(1,317)	1:101:A:LEU:HD11	2:201:A:Z90:HAI	2	0.14	0.0	0.14
(1,317)	1:101:A:LEU:HD12	2:201:A:Z90:HAI	2	0.14	0.0	0.14
(1,317)	1:101:A:LEU:HD13	2:201:A:Z90:HAI	2	0.14	0.0	0.14
(1,1163)	1:153:A:VAL:HG11	1:153:A:VAL:H	2	0.14	0.04	0.14
(1,1163)	1:153:A:VAL:HG12	1:153:A:VAL:H	2	0.14	0.04	0.14
(1,1163)	1:153:A:VAL:HG13	1:153:A:VAL:H	2	0.14	0.04	0.14
(1,1497)	1:80:A:GLU:HB2	1:82:A:GLY:H	2	0.14	0.0	0.14
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD11	2	0.14	0.02	0.14
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD12	2	0.14	0.02	0.14
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD13	2	0.14	0.02	0.14
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG11	2	0.12	0.0	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG12	2	0.12	0.0	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG13	2	0.12	0.0	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG21	2	0.12	0.0	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG22	2	0.12	0.0	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG23	2	0.12	0.0	0.12

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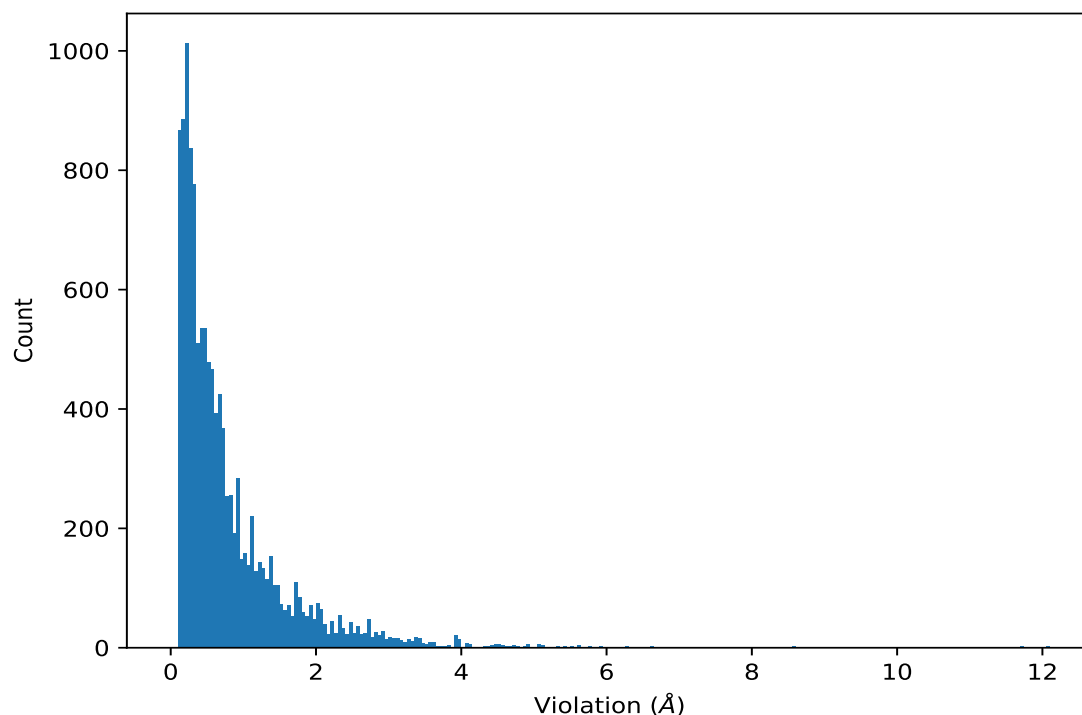
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,944)	1:162:A:ILE:HD11	1:164:A:MET:H	2	0.12	0.0	0.12
(1,944)	1:162:A:ILE:HD12	1:164:A:MET:H	2	0.12	0.0	0.12
(1,944)	1:162:A:ILE:HD13	1:164:A:MET:H	2	0.12	0.0	0.12
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD11	2	0.12	0.0	0.12
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD12	2	0.12	0.0	0.12
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD13	2	0.12	0.0	0.12

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

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

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

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



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

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



Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	5	12.06
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	5	12.06
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	10	11.71
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	10	11.71
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	1	8.59
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	1	8.59
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	8	6.62
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	8	6.62
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	9	6.26
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	9	6.26
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	6	5.93
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	6	5.93
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	5	5.75
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	5	5.75
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	5	5.75
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	6	5.61
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	6	5.61
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	4	5.6
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	4	5.6
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	8	5.59
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	4	5.51
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	4	5.51
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	6	5.44
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	6	5.44
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	6	5.44
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	7	5.35
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	9	5.3
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	9	5.3
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	6	5.11
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	6	5.11
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	6	5.11
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD1	7	5.1
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD2	7	5.1
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	6	5.08
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	6	5.08
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	6	5.08
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	5	5.07
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	5	5.07
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	5	5.07
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	1	5.02
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	5	4.94
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	5	4.94
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	5	4.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	9	4.93
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	9	4.93
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	9	4.93
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	1	4.87
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	1	4.87
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	1	4.87
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	1	4.76
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	1	4.76
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	1	4.76
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	9	4.73
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	9	4.73
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	1	4.72
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	1	4.72
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	1	4.72
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE1	6	4.68
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE2	6	4.68
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE3	6	4.68
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	4	4.61
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	4	4.61
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	4	4.61
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	7	4.58
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	7	4.58
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	5	4.58
(1,2017)	1:136:A:TYR:HB2	1:119:A:SER:H	7	4.56
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	2	4.53
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	2	4.53
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	2	4.53
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	4	4.5
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	4	4.5
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	4	4.5
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	9	4.49
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	9	4.49
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	9	4.49
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	5	4.47
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	5	4.47
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	5	4.47
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	6	4.42
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	6	4.42
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	3	4.41
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	3	4.41
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	6	4.36
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	6	4.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	6	4.36
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	9	4.31
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	9	4.31
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	4	4.14
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	3	4.13
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	3	4.13
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	10	4.11
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	3	4.11
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	3	4.11
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	1	4.09
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	1	4.09
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	1	4.09
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	10	4.06
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	4	4.05
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	4	4.05
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	4	4.05
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	5	4.02
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	4	3.99
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	1	3.97
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	1	3.97
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	1	3.97
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	1	3.96
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	1	3.96
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	1	3.96
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	5	3.95
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	5	3.95
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	5	3.95
(1,622)	1:140:A:GLU:HB3	1:170:A:ARG:H	7	3.95
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	9	3.95
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	9	3.95
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	9	3.95
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	1	3.94
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	1	3.94
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	1	3.94
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	1	3.92
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	1	3.92
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	1	3.92
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	1	3.92
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	1	3.92
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	1	3.92
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	1	3.92
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	1	3.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	1	3.92
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	1	3.92
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	1	3.92
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	1	3.92
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	1	3.92
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	1	3.92
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	1	3.92
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	1	3.92
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	1	3.92
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	1	3.92
(1,622)	1:140:A:GLU:HB3	1:170:A:ARG:H	9	3.86
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	10	3.82
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	10	3.82
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	10	3.82
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE1	10	3.81
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE2	10	3.81
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	2	3.79
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD1	2	3.76
(1,1620)	2:201:A:Z90:HAJ	1:83:A:TYR:HD2	2	3.76
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	4	3.71
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	4	3.71
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	10	3.68
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	10	3.68
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	10	3.68
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	1	3.63
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	1	3.63
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	1	3.63
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	10	3.62
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	10	3.62
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	10	3.62
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	1	3.6
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	1	3.6
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	1	3.6
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	8	3.58
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	9	3.58
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	9	3.58
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	9	3.58
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	1	3.56
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	1	3.56
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	1	3.56
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	7	3.56
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	7	3.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	7	3.56
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	6	3.54
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	6	3.54
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	9	3.53
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	9	3.53
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	9	3.53
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	1	3.5
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	2	3.49
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	10	3.47
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	10	3.47
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	10	3.47
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	1	3.45
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	1	3.45
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	1	3.45
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	10	3.43
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	4	3.43
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	4	3.43
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	4	3.43
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD11	4	3.42
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD12	4	3.42
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD13	4	3.42
(1,3044)	1:136:A:TYR:HD1	1:119:A:SER:H	7	3.42
(1,3044)	1:136:A:TYR:HD2	1:119:A:SER:H	7	3.42
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	8	3.41
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	8	3.41
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	8	3.41
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	6	3.4
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	3	3.4
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	3	3.4
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	3	3.4
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	6	3.38
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	1	3.38
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	1	3.38
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	2	3.37
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	2	3.37
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	2	3.37
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	5	3.36
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	5	3.36
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	5	3.36
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	7	3.36
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	7	3.36
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	7	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	5	3.36
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	5	3.36
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	5	3.36
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	7	3.36
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	7	3.36
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	2	3.34
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	2	3.34
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	3	3.33
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	9	3.32
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	9	3.32
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	9	3.32
(1,622)	1:140:A:GLU:HB3	1:170:A:ARG:H	6	3.31
(1,3456)	1:158:A:HIS:HD2	1:94:A:VAL:HA	10	3.3
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	6	3.3
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	6	3.3
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	6	3.3
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	3	3.29
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	3	3.29
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	3	3.29
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	2	3.28
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	2	3.28
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	5	3.26
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	5	3.26
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	5	3.26
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE1	1	3.26
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE2	1	3.26
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE3	1	3.26
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	10	3.26
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	10	3.26
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	10	3.26
(1,2771)	1:137:A:SER:HA	1:119:A:SER:H	9	3.24
(1,1992)	1:92:A:SER:HB2	1:93:A:ASN:HD22	3	3.24
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	7	3.22
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	9	3.22
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	9	3.22
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	9	3.22
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	8	3.21
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE1	1	3.2
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE2	1	3.2
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE3	1	3.2
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	9	3.19
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	9	3.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	9	3.18
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	9	3.18
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	9	3.17
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	10	3.16
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	5	3.16
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	5	3.16
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	5	3.16
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	7	3.15
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	4	3.15
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	4	3.15
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	4	3.15
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	5	3.14
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	7	3.14
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	4	3.14
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	4	3.14
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	4	3.14
(1,998)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	10	3.14
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	7	3.14
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	7	3.14
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	7	3.14
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	4	3.13
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	9	3.12
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	5	3.11
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	5	3.11
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	5	3.11
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	9	3.11
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	9	3.1
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	1	3.09
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	1	3.09
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	6	3.09
(1,1565)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	10	3.09
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	10	3.08
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	10	3.08
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	10	3.06
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	10	3.06
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	10	3.06
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	9	3.06
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	9	3.06
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	9	3.06
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	8	3.05
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	8	3.05
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	2	3.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	6	3.05
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	6	3.04
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	1	3.03
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	1	3.03
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	1	3.03
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	7	3.03
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	7	3.03
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	7	3.03
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	4	3.03
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	4	3.03
(1,2460)	1:138:A:GLU:H	1:118:A:PRO:HA	1	3.02
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	7	3.02
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	7	3.02
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	7	3.02
(1,1874)	1:170:A:ARG:HE	1:177:A:THR:H	3	3.01
(1,1014)	1:174:A:CYS:HB2	1:169:A:GLN:H	9	3.0
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	4	3.0
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	4	3.0
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	4	3.0
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	8	2.99
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	8	2.99
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	8	2.98
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	8	2.98
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	8	2.98
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	8	2.98
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	8	2.98
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	8	2.98
(1,1019)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	10	2.98
(1,2771)	1:137:A:SER:HA	1:119:A:SER:H	2	2.96
(1,2460)	1:138:A:GLU:H	1:118:A:PRO:HA	6	2.96
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	4	2.95
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	4	2.95
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	4	2.95
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	5	2.94
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD21	1	2.94
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD22	1	2.94
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD23	1	2.94
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	3	2.94
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	3	2.94
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	3	2.94
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	3	2.94
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	3	2.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	3	2.94
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	3	2.94
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	3	2.94
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	3	2.94
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	10	2.93
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	10	2.93
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	10	2.93
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	6	2.93
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	6	2.93
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	6	2.93
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	6	2.91
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	5	2.91
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	5	2.91
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	5	2.91
(1,450)	1:155:A:GLN:HG3	1:159:A:GLY:H	6	2.9
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	2	2.9
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	2	2.9
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	2	2.9
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	4	2.89
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	4	2.89
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	4	2.89
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	6	2.89
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	6	2.89
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	6	2.89
(1,420)	1:136:A:TYR:HB3	1:119:A:SER:H	7	2.89
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	3	2.89
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	3	2.89
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	5	2.88
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	5	2.88
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	9	2.87
(1,3456)	1:158:A:HIS:HD2	1:94:A:VAL:HA	9	2.86
(1,1874)	1:170:A:ARG:HE	1:177:A:THR:H	7	2.86
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	2	2.86
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	2	2.86
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	2	2.86
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	8	2.85
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	8	2.85
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	8	2.85
(1,1146)	1:100:A:ASN:HD22	1:99:A:GLN:H	9	2.85
(1,1874)	1:170:A:ARG:HE	1:177:A:THR:H	9	2.84
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	6	2.84
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	6	2.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	6	2.84
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	6	2.84
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	6	2.84
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	6	2.84
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	6	2.84
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	6	2.84
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	6	2.84
(1,2711)	1:108:A:LEU:HD11	1:111:A:ILE:HB	10	2.83
(1,2711)	1:108:A:LEU:HD12	1:111:A:ILE:HB	10	2.83
(1,2711)	1:108:A:LEU:HD13	1:111:A:ILE:HB	10	2.83
(1,2711)	1:108:A:LEU:HD21	1:111:A:ILE:HB	10	2.83
(1,2711)	1:108:A:LEU:HD22	1:111:A:ILE:HB	10	2.83
(1,2711)	1:108:A:LEU:HD23	1:111:A:ILE:HB	10	2.83
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	4	2.83
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	6	2.82
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	10	2.81
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	10	2.81
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	10	2.81
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	7	2.81
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	7	2.81
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	7	2.81
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	7	2.8
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	5	2.8
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG21	6	2.79
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG22	6	2.79
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG23	6	2.79
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	1	2.79
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG21	6	2.79
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG22	6	2.79
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG23	6	2.79
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	3	2.79
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	3	2.79
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	3	2.79
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	7	2.78
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	7	2.78
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	7	2.78
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	4	2.77
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	5	2.76
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	3	2.76
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	3	2.76
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	10	2.75
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	5	2.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD11	7	2.74
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD12	7	2.74
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD13	7	2.74
(1,558)	1:125:A:ALA:HA	1:132:A:ILE:HG13	3	2.74
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	5	2.74
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	5	2.74
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	5	2.74
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD1	6	2.73
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD2	6	2.73
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD1	6	2.73
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD2	6	2.73
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD1	6	2.73
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD2	6	2.73
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	1	2.73
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	1	2.73
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	1	2.73
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	1	2.73
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	2	2.73
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	2	2.73
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	2	2.73
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	9	2.73
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	9	2.73
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	9	2.73
(2,1)	1:135:A:TYR:HH	2:201:A:Z90:OAC	7	2.72
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	5	2.72
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	5	2.72
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	9	2.72
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	9	2.71
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	9	2.71
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	9	2.71
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	8	2.71
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	8	2.71
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	8	2.71
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	8	2.71
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	8	2.71
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	8	2.71
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	4	2.7
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	4	2.7
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	4	2.7
(1,2125)	1:136:A:TYR:HA	1:119:A:SER:H	7	2.7
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	6	2.7
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	6	2.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1927)	1:120:A:PHE:HE1	1:119:A:SER:H	10	2.7
(1,1927)	1:120:A:PHE:HE2	1:119:A:SER:H	10	2.7
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	7	2.7
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	7	2.7
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	7	2.7
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	5	2.69
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	5	2.69
(1,2301)	1:136:A:TYR:HA	1:119:A:SER:H	7	2.69
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	1	2.69
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	1	2.69
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	1	2.69
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	1	2.69
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	1	2.69
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	1	2.69
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	1	2.69
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	1	2.69
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	1	2.69
(1,1146)	1:100:A:ASN:HD22	1:99:A:GLN:H	10	2.68
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	2	2.67
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	2	2.67
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	2	2.67
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	7	2.66
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	7	2.66
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	5	2.66
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	5	2.66
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	9	2.66
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	9	2.66
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	9	2.66
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	2	2.65
(1,1617)	1:49:A:TYR:HE1	1:48:A:THR:H	2	2.64
(1,1617)	1:49:A:TYR:HE2	1:48:A:THR:H	2	2.64
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE1	3	2.64
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE2	3	2.64
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE3	3	2.64
(1,998)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	9	2.63
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	5	2.62
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	9	2.62
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	9	2.62
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	6	2.62
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	6	2.62
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	6	2.62
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	10	2.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	10	2.62
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	10	2.62
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE1	2	2.61
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE2	2	2.61
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE3	2	2.61
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	3	2.6
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD11	9	2.6
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD12	9	2.6
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD13	9	2.6
(1,1146)	1:100:A:ASN:HD22	1:99:A:GLN:H	5	2.6
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD1	2	2.59
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD2	2	2.59
(1,1014)	1:174:A:CYS:HB2	1:169:A:GLN:H	7	2.59
(1,307)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	3	2.59
(1,307)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	3	2.59
(1,307)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	3	2.59
(1,307)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	6	2.59
(1,307)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	6	2.59
(1,307)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	6	2.59
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	9	2.59
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	9	2.59
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	9	2.59
(1,2125)	1:136:A:TYR:HA	1:119:A:SER:H	9	2.58
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	10	2.58
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	10	2.58
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	10	2.58
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	3	2.58
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	3	2.58
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	3	2.58
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	3	2.58
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	3	2.58
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	3	2.58
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	9	2.57
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	9	2.57
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	9	2.57
(1,2301)	1:136:A:TYR:HA	1:119:A:SER:H	9	2.57
(1,1565)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	9	2.57
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	3	2.57
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	3	2.57
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	3	2.57
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	3	2.56
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	3	2.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	3	2.56
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE1	9	2.56
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE2	9	2.56
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE3	9	2.56
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	4	2.54
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	2	2.54
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	5	2.53
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	5	2.53
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	5	2.53
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	5	2.53
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	5	2.53
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	10	2.53
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	10	2.53
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	10	2.53
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	9	2.52
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	9	2.52
(1,3311)	1:158:A:HIS:HD2	1:157:A:ILE:HG12	9	2.52
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	8	2.52
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	8	2.52
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	8	2.52
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	5	2.51
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	5	2.51
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	5	2.51
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	10	2.5
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	10	2.5
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	10	2.5
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	10	2.5
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	10	2.5
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	10	2.5
(1,2513)	1:142:A:LEU:HD21	1:139:A:ARG:H	8	2.49
(1,2513)	1:142:A:LEU:HD22	1:139:A:ARG:H	8	2.49
(1,2513)	1:142:A:LEU:HD23	1:139:A:ARG:H	8	2.49
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	1	2.49
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	1	2.49
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	1	2.49
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	1	2.49
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	1	2.49
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	1	2.49
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	5	2.49
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	5	2.49
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	5	2.49
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	5	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	5	2.49
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	5	2.49
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	5	2.49
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	6	2.49
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	6	2.49
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	6	2.49
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	2	2.48
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	2	2.48
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	2	2.48
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	5	2.48
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	5	2.48
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	5	2.48
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	3	2.48
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	3	2.48
(1,1019)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	9	2.47
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	1	2.46
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	7	2.46
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	7	2.46
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	7	2.46
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	3	2.46
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	3	2.46
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	3	2.46
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	6	2.45
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	9	2.45
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	9	2.45
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	9	2.45
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	2	2.45
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	2	2.45
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	2	2.45
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	1	2.44
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	1	2.44
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	9	2.44
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE1	1	2.44
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE2	1	2.44
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	1	2.44
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	6	2.43
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	6	2.43
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	6	2.43
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	6	2.41
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	6	2.41
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	3	2.41
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	3	2.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	6	2.41
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	6	2.41
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	6	2.41
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	3	2.41
(1,2460)	1:138:A:GLU:H	1:118:A:PRO:HA	2	2.41
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	1	2.41
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	1	2.41
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	1	2.41
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	8	2.4
(1,524)	1:124:A:ASP:HB2	1:131:A:LEU:H	2	2.4
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	3	2.39
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	3	2.39
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	3	2.39
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	2	2.39
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	2	2.39
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	2	2.39
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	9	2.39
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	9	2.39
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	9	2.39
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	9	2.38
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	9	2.38
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	9	2.38
(1,1396)	1:158:A:HIS:HD2	1:154:A:ALA:HA	10	2.38
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	7	2.38
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	7	2.38
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	7	2.38
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	7	2.38
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	1	2.38
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	4	2.36
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	4	2.36
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	4	2.36
(1,1113)	1:49:A:TYR:HE1	1:46:A:SER:H	2	2.36
(1,1113)	1:49:A:TYR:HE2	1:46:A:SER:H	2	2.36
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	4	2.36
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	4	2.36
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	4	2.36
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	5	2.35
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG21	10	2.35
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG22	10	2.35
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG23	10	2.35
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD11	9	2.35
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD12	9	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD13	9	2.35
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	5	2.34
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	5	2.34
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	5	2.34
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	5	2.33
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	4	2.32
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	3	2.32
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	8	2.32
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	8	2.32
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	8	2.32
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE1	1	2.32
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE2	1	2.32
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE3	1	2.32
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	8	2.32
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	8	2.32
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	8	2.32
(1,307)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	7	2.32
(1,307)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	7	2.32
(1,307)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	7	2.32
(1,307)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	9	2.32
(1,307)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	9	2.32
(1,307)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	9	2.32
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	4	2.31
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	8	2.31
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	8	2.31
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	8	2.31
(1,254)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	3	2.31
(1,254)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	3	2.31
(1,254)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	3	2.31
(1,254)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	6	2.31
(1,254)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	6	2.31
(1,254)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	6	2.31
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	1	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	1	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	1	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	2	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	2	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	2	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	6	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	6	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	6	2.3
(1,2460)	1:138:A:GLU:H	1:118:A:PRO:HA	9	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	2	2.3
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	8	2.3
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	8	2.3
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	8	2.3
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	8	2.3
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	8	2.3
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	8	2.3
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	8	2.3
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	8	2.3
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	8	2.3
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	8	2.3
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	5	2.3
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	5	2.3
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	5	2.3
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	8	2.29
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	8	2.29
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	8	2.29
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	3	2.29
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	4	2.29
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	4	2.29
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	4	2.29
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	1	2.28
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	4	2.27
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	4	2.27
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	7	2.27
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	7	2.27
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	7	2.27
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	7	2.27
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	7	2.27
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	7	2.27
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	7	2.27
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	7	2.27
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	7	2.27
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE1	5	2.26
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE2	5	2.26
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	9	2.26
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	9	2.26
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	9	2.26
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	6	2.25
(1,1992)	1:92:A:SER:HB2	1:93:A:ASN:HD22	7	2.24
(1,1456)	1:160:A:THR:HB	1:158:A:HIS:H	6	2.24
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	10	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	10	2.24
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	10	2.24
(1,2822)	1:137:A:SER:HB2	1:139:A:ARG:H	6	2.23
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	9	2.23
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	9	2.23
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	9	2.23
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	10	2.23
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	10	2.23
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	10	2.23
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	10	2.22
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	10	2.22
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	10	2.22
(1,2513)	1:142:A:LEU:HD21	1:139:A:ARG:H	4	2.22
(1,2513)	1:142:A:LEU:HD22	1:139:A:ARG:H	4	2.22
(1,2513)	1:142:A:LEU:HD23	1:139:A:ARG:H	4	2.22
(1,2316)	1:171:A:ASN:HB2	1:174:A:CYS:HB3	6	2.22
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG11	6	2.22
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG12	6	2.22
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG13	6	2.22
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG11	6	2.22
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG12	6	2.22
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG13	6	2.22
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG11	6	2.22
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG12	6	2.22
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG13	6	2.22
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE1	10	2.22
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE2	10	2.22
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE3	10	2.22
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	4	2.21
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	8	2.21
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	8	2.21
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	8	2.21
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	3	2.21
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE1	10	2.2
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE2	10	2.2
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE3	10	2.2
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	10	2.2
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	10	2.2
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	10	2.2
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	2	2.2
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	2	2.2
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	4	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	4	2.19
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	4	2.19
(1,3311)	1:158:A:HIS:HD2	1:157:A:ILE:HG12	1	2.18
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	5	2.18
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	5	2.18
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	6	2.18
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	6	2.18
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	6	2.18
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	6	2.17
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	7	2.16
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	7	2.16
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	7	2.16
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	1	2.16
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	7	2.15
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	7	2.15
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	7	2.15
(1,2513)	1:142:A:LEU:HD21	1:139:A:ARG:H	2	2.15
(1,2513)	1:142:A:LEU:HD22	1:139:A:ARG:H	2	2.15
(1,2513)	1:142:A:LEU:HD23	1:139:A:ARG:H	2	2.15
(1,1874)	1:170:A:ARG:HE	1:177:A:THR:H	10	2.15
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	7	2.15
(1,498)	1:176:A:HIS:HD2	1:178:A:GLN:H	4	2.15
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	7	2.14
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	7	2.14
(1,2316)	1:171:A:ASN:HB2	1:174:A:CYS:HB3	2	2.14
(1,2188)	1:183:A:GLU:HB2	1:185:A:GLU:H	8	2.14
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	10	2.14
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	7	2.14
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	3	2.13
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	4	2.13
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	8	2.13
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	8	2.13
(1,2701)	1:99:A:GLN:HE22	1:95:A:ARG:HG3	6	2.12
(1,2644)	1:59:A:LEU:HD11	1:55:A:ALA:H	2	2.12
(1,2644)	1:59:A:LEU:HD12	1:55:A:ALA:H	2	2.12
(1,2644)	1:59:A:LEU:HD13	1:55:A:ALA:H	2	2.12
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	7	2.12
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	7	2.12
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	8	2.11
(1,3234)	1:100:A:ASN:HD22	1:96:A:GLU:HB3	5	2.1
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG21	5	2.1
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG22	5	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG23	5	2.1
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	10	2.1
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	10	2.1
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	10	2.1
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD21	3	2.1
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD22	3	2.1
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD23	3	2.1
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	4	2.1
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	4	2.1
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	4	2.1
(1,1704)	1:184:A:LYS:HD2	1:161:A:GLU:H	3	2.1
(1,1704)	1:184:A:LYS:HD3	1:161:A:GLU:H	3	2.1
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG21	5	2.1
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG22	5	2.1
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG23	5	2.1
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	2	2.1
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	2	2.1
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	8	2.1
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	8	2.1
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	8	2.1
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	2	2.09
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	2	2.09
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	2	2.09
(1,1988)	1:26:A:LYS:HB3	1:23:A:GLU:H	7	2.09
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	10	2.09
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	10	2.09
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	6	2.08
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	5	2.08
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	5	2.08
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	5	2.08
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	9	2.08
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	9	2.08
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	9	2.08
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	8	2.08
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	8	2.08
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	8	2.08
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	8	2.08
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	8	2.08
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	8	2.08
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	8	2.08
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	8	2.08
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	8	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	5	2.07
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	5	2.07
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	5	2.07
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	5	2.07
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	5	2.07
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	5	2.07
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	5	2.07
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	5	2.07
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	5	2.07
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	3	2.07
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	3	2.07
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	3	2.07
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	3	2.07
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	3	2.07
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	3	2.07
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	4	2.07
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	4	2.07
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	4	2.07
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD11	3	2.07
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD12	3	2.07
(1,884)	1:78:A:CYS:HB3	1:11:A:LEU:HD13	3	2.07
(1,273)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	3	2.07
(1,273)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	3	2.07
(1,273)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	3	2.07
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	1	2.07
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	1	2.07
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	1	2.07
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	1	2.07
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	1	2.07
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	1	2.07
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	8	2.06
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	2	2.06
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	2	2.06
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	2	2.06
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:H	10	2.06
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:H	10	2.06
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:H	10	2.06
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	8	2.05
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	8	2.05
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	8	2.05
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	4	2.05
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	4	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	4	2.05
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD21	6	2.04
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD22	6	2.04
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD23	6	2.04
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD21	6	2.04
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD22	6	2.04
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD23	6	2.04
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD21	6	2.04
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD22	6	2.04
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD23	6	2.04
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD1	6	2.04
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD2	6	2.04
(1,2479)	1:92:A:SER:HB3	1:93:A:ASN:HD22	8	2.04
(1,2289)	1:158:A:HIS:HB3	1:160:A:THR:H	5	2.04
(1,254)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	7	2.04
(1,254)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	7	2.04
(1,254)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	7	2.04
(1,254)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	9	2.04
(1,254)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	9	2.04
(1,254)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	9	2.04
(1,2701)	1:99:A:GLN:HE22	1:95:A:ARG:HG3	5	2.03
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	10	2.03
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	10	2.03
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	10	2.03
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	10	2.03
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	10	2.03
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	10	2.03
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	10	2.03
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	10	2.03
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	10	2.03
(1,2340)	1:139:A:ARG:HG2	1:141:A:GLY:H	2	2.03
(1,1936)	1:175:A:ASP:H	1:171:A:ASN:H	8	2.03
(1,1874)	1:170:A:ARG:HE	1:177:A:THR:H	1	2.03
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	1	2.03
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	1	2.02
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	1	2.02
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	1	2.02
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	1	2.02
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	1	2.02
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	10	2.02
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	10	2.02
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	10	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	10	2.02
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	10	2.02
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	10	2.02
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	10	2.02
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	10	2.02
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	10	2.02
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	5	2.02
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	4	2.02
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	4	2.02
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	4	2.02
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	1	2.02
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	1	2.02
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	1	2.02
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD11	6	2.01
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD12	6	2.01
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD13	6	2.01
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD11	6	2.01
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD12	6	2.01
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD13	6	2.01
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD11	6	2.01
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD12	6	2.01
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD13	6	2.01
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	1	2.01
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	1	2.01
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	1	2.01
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	4	2.01
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	8	2.01
(1,2169)	1:186:A:SER:H	1:184:A:LYS:HA	5	2.01
(1,1835)	1:58:A:VAL:H	1:59:A:LEU:HG	2	2.01
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	3	2.01
(1,2315)	1:159:A:GLY:H	1:157:A:ILE:H	6	2.0
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	6	2.0
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	6	2.0
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	6	2.0
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	4	1.99
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	4	1.99
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD11	9	1.99
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD12	9	1.99
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD13	9	1.99
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD21	9	1.99
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD22	9	1.99
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD23	9	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1187)	1:31:A:LEU:HA	1:35:A:GLY:H	3	1.99
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	2	1.98
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	10	1.98
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	10	1.98
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	10	1.98
(1,1396)	1:158:A:HIS:HD2	1:154:A:ALA:HA	9	1.98
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG11	5	1.97
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG12	5	1.97
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG13	5	1.97
(1,1494)	1:176:A:HIS:H	1:174:A:CYS:HB2	7	1.97
(1,1494)	1:176:A:HIS:H	1:174:A:CYS:HB2	9	1.97
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	10	1.97
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG11	10	1.97
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG12	10	1.97
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG13	10	1.97
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG11	10	1.97
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG12	10	1.97
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG13	10	1.97
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG11	10	1.97
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG12	10	1.97
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG13	10	1.97
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	2	1.97
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	3	1.97
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	7	1.97
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	7	1.97
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	7	1.97
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	7	1.97
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	7	1.97
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	7	1.97
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	7	1.97
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	7	1.97
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	7	1.97
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	4	1.96
(1,1956)	1:34:A:GLU:HB2	1:36:A:GLN:H	8	1.96
(1,1956)	1:34:A:GLU:HB3	1:36:A:GLN:H	8	1.96
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	6	1.96
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE1	6	1.95
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE2	6	1.95
(1,730)	1:22:A:TRP:HH2	1:26:A:LYS:HB2	7	1.95
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD21	10	1.94
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD22	10	1.94
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD23	10	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD21	1	1.94
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD22	1	1.94
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD23	1	1.94
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD21	1	1.94
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD22	1	1.94
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD23	1	1.94
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD21	1	1.94
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD22	1	1.94
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD23	1	1.94
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	4	1.94
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	8	1.94
(1,525)	1:131:A:LEU:HB2	1:183:A:GLU:H	3	1.94
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	8	1.93
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	8	1.93
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	8	1.93
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	7	1.93
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	7	1.93
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	7	1.93
(1,3456)	1:158:A:HIS:HD2	1:94:A:VAL:HA	5	1.92
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	8	1.92
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	1	1.92
(1,1704)	1:184:A:LYS:HD2	1:161:A:GLU:H	10	1.92
(1,1704)	1:184:A:LYS:HD3	1:161:A:GLU:H	10	1.92
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	9	1.92
(1,316)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	4	1.92
(1,316)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	4	1.92
(1,316)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	4	1.92
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:H	8	1.92
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:H	8	1.92
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:H	8	1.92
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	10	1.91
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	10	1.91
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD21	7	1.91
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD22	7	1.91
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD23	7	1.91
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD21	7	1.91
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD22	7	1.91
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD23	7	1.91
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD21	7	1.91
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD22	7	1.91
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD23	7	1.91
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	5	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	5	1.91
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	5	1.91
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	3	1.91
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	3	1.91
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	3	1.91
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD11	8	1.91
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD12	8	1.91
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD13	8	1.91
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	9	1.91
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	9	1.91
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	9	1.91
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	2	1.91
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	2	1.91
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	2	1.91
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:H	5	1.91
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:H	5	1.91
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:H	5	1.91
(1,2237)	1:120:A:PHE:HA	1:135:A:TYR:H	2	1.9
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	3	1.9
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	3	1.9
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	1	1.9
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	1	1.9
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	1	1.9
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	4	1.9
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	4	1.9
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	4	1.9
(1,2485)	1:30:A:GLN:HE22	1:28:A:GLU:HA	10	1.89
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	1	1.89
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	9	1.89
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	9	1.89
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	9	1.89
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	4	1.89
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	4	1.89
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	4	1.89
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	2	1.88
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	2	1.88
(1,1797)	1:175:A:ASP:H	1:171:A:ASN:H	8	1.88
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	9	1.88
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	9	1.88
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	9	1.88
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD11	3	1.87
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD12	3	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD13	3	1.87
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	2	1.87
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	8	1.87
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	8	1.87
(1,2701)	1:99:A:GLN:HE22	1:95:A:ARG:HG3	1	1.87
(1,2485)	1:30:A:GLN:HE22	1:28:A:GLU:HA	2	1.87
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	6	1.87
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	5	1.87
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	6	1.87
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	6	1.87
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	6	1.87
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG11	1	1.87
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG12	1	1.87
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG13	1	1.87
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG11	1	1.87
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG12	1	1.87
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG13	1	1.87
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG11	1	1.87
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG12	1	1.87
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG13	1	1.87
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	1	1.87
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	3	1.87
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	3	1.87
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	3	1.87
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	5	1.86
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	5	1.86
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	5	1.86
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	7	1.86
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	7	1.86
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	7	1.86
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	4	1.86
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	4	1.86
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	4	1.86
(1,1704)	1:184:A:LYS:HD2	1:161:A:GLU:H	9	1.85
(1,1704)	1:184:A:LYS:HD3	1:161:A:GLU:H	9	1.85
(1,622)	1:140:A:GLU:HB3	1:170:A:ARG:H	2	1.85
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	10	1.85
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	7	1.84
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	7	1.84
(1,2449)	1:169:A:GLN:HE22	1:168:A:GLN:HA	2	1.84
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	7	1.84
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	8	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:174:A:CYS:HB2	1:169:A:GLN:H	10	1.84
(1,3526)	1:12:A:LEU:HA	1:16:A:ASN:HD22	3	1.83
(1,3311)	1:158:A:HIS:HD2	1:157:A:ILE:HG12	6	1.83
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	9	1.83
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	1	1.83
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	1	1.83
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	1	1.83
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	7	1.83
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	7	1.83
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	7	1.83
(1,1810)	1:93:A:ASN:HD22	1:96:A:GLU:HB3	7	1.83
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	5	1.83
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	8	1.83
(1,524)	1:124:A:ASP:HB2	1:131:A:LEU:H	3	1.83
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	8	1.83
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	8	1.83
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	8	1.83
(1,2771)	1:137:A:SER:HA	1:119:A:SER:H	6	1.82
(1,2485)	1:30:A:GLN:HE22	1:28:A:GLU:HA	4	1.82
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	3	1.82
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	7	1.82
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	7	1.82
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	7	1.82
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	4	1.81
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	4	1.81
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	4	1.81
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	4	1.81
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	4	1.81
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	4	1.81
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	4	1.81
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	4	1.81
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	4	1.81
(1,2479)	1:92:A:SER:HB3	1:93:A:ASN:HD22	3	1.81
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	8	1.81
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE1	6	1.81
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE2	6	1.81
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	6	1.81
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	8	1.81
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	2	1.81
(1,3234)	1:100:A:ASN:HD22	1:96:A:GLU:HB3	10	1.8
(1,2485)	1:30:A:GLN:HE22	1:28:A:GLU:HA	5	1.8
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	2	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	6	1.8
(1,1992)	1:92:A:SER:HB2	1:93:A:ASN:HD22	8	1.8
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD11	4	1.8
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD12	4	1.8
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD13	4	1.8
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD21	4	1.8
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD22	4	1.8
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD23	4	1.8
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	1	1.8
(1,265)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	4	1.8
(1,265)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	4	1.8
(1,265)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	4	1.8
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	8	1.79
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	5	1.79
(1,1187)	1:31:A:LEU:HA	1:35:A:GLY:H	10	1.79
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	2	1.79
(1,332)	2:201:A:Z90:HAR	1:117:A:ALA:HA	8	1.79
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD11	3	1.78
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD12	3	1.78
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD13	3	1.78
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD11	3	1.78
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD12	3	1.78
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD13	3	1.78
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD11	3	1.78
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD12	3	1.78
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD13	3	1.78
(1,1396)	1:158:A:HIS:HD2	1:154:A:ALA:HA	5	1.78
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	2	1.77
(1,1439)	1:99:A:GLN:HE22	1:95:A:ARG:HG2	9	1.77
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	5	1.77
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	5	1.77
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	5	1.77
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	7	1.77
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	7	1.77
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	7	1.77
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	2	1.77
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	2	1.77
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	2	1.77
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	2	1.77
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	2	1.77
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	2	1.77
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	6	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	6	1.76
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	6	1.76
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	6	1.76
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	6	1.76
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	6	1.76
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	6	1.76
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	6	1.76
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	6	1.76
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	5	1.76
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	5	1.76
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	5	1.76
(1,2311)	1:104:A:LEU:HD11	1:90:A:LEU:HD21	7	1.76
(1,2311)	1:104:A:LEU:HD11	1:90:A:LEU:HD22	7	1.76
(1,2311)	1:104:A:LEU:HD11	1:90:A:LEU:HD23	7	1.76
(1,2311)	1:104:A:LEU:HD12	1:90:A:LEU:HD21	7	1.76
(1,2311)	1:104:A:LEU:HD12	1:90:A:LEU:HD22	7	1.76
(1,2311)	1:104:A:LEU:HD12	1:90:A:LEU:HD23	7	1.76
(1,2311)	1:104:A:LEU:HD13	1:90:A:LEU:HD21	7	1.76
(1,2311)	1:104:A:LEU:HD13	1:90:A:LEU:HD22	7	1.76
(1,2311)	1:104:A:LEU:HD13	1:90:A:LEU:HD23	7	1.76
(1,1927)	1:120:A:PHE:HE1	1:119:A:SER:H	3	1.76
(1,1927)	1:120:A:PHE:HE2	1:119:A:SER:H	3	1.76
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE1	10	1.76
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE2	10	1.76
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE3	10	1.76
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE1	10	1.76
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE2	10	1.76
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE3	10	1.76
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE1	10	1.76
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE2	10	1.76
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE3	10	1.76
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	10	1.76
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	10	1.76
(1,3121)	1:41:A:ILE:HB	1:3:A:GLY:H	7	1.75
(1,2188)	1:183:A:GLU:HB2	1:185:A:GLU:H	6	1.75
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	2	1.75
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	2	1.75
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	2	1.75
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD21	1	1.75
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD22	1	1.75
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD23	1	1.75
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD21	1	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD22	1	1.75
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD23	1	1.75
(1,1104)	1:169:A:GLN:HE22	1:168:A:GLN:HA	2	1.75
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	1	1.75
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	1	1.75
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	1	1.75
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	6	1.75
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	6	1.75
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	6	1.75
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	6	1.75
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	3	1.75
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	3	1.75
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	3	1.75
(1,3463)	1:170:A:ARG:HE	1:176:A:HIS:H	3	1.74
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	9	1.74
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	9	1.74
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	9	1.74
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	9	1.74
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	9	1.74
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	9	1.74
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	9	1.74
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	9	1.74
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	9	1.74
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	9	1.74
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	10	1.74
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	9	1.74
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	9	1.74
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	9	1.74
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	3	1.74
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	3	1.74
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	3	1.74
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	2	1.74
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	2	1.74
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	2	1.74
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	2	1.74
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	2	1.74
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	2	1.74
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	2	1.74
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	2	1.74
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	2	1.74
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	1	1.74
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	1	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	1	1.74
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	8	1.74
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	8	1.74
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	8	1.74
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	7	1.74
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	7	1.74
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	7	1.74
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	10	1.73
(1,3311)	1:158:A:HIS:HD2	1:157:A:ILE:HG12	5	1.73
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD11	10	1.73
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD12	10	1.73
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD13	10	1.73
(1,1439)	1:99:A:GLN:HE22	1:95:A:ARG:HG2	6	1.73
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	9	1.73
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	9	1.73
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	9	1.73
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	10	1.72
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	10	1.72
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	10	1.72
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	1	1.72
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	1	1.72
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	1	1.72
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	1	1.72
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	1	1.72
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	1	1.72
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	1	1.72
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	1	1.72
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	1	1.72
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB1	1	1.72
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB2	1	1.72
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB3	1	1.72
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	6	1.72
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	6	1.72
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	6	1.72
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	6	1.72
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	6	1.72
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	6	1.72
(1,420)	1:136:A:TYR:HB3	1:119:A:SER:H	9	1.72
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	1	1.72
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	1	1.72
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	1	1.72
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	9	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	9	1.72
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	9	1.72
(1,3573)	1:22:A:TRP:HE3	1:26:A:LYS:HB2	7	1.71
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	8	1.71
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	8	1.71
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	8	1.71
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	8	1.71
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	8	1.71
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	8	1.71
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	8	1.71
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	8	1.71
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	8	1.71
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	7	1.71
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	7	1.71
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	7	1.71
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	2	1.71
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	2	1.71
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	2	1.71
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	1	1.71
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	2	1.71
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	2	1.71
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	4	1.71
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	4	1.71
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	4	1.71
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD11	4	1.7
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD12	4	1.7
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD13	4	1.7
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD11	4	1.7
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD12	4	1.7
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD13	4	1.7
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD11	4	1.7
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD12	4	1.7
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD13	4	1.7
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	3	1.7
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	7	1.7
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	2	1.7
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	2	1.7
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	2	1.7
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	4	1.69
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD11	4	1.69
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD12	4	1.69
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD13	4	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	6	1.69
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	10	1.69
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	10	1.69
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	10	1.69
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	3	1.68
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	3	1.68
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	10	1.68
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	6	1.67
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	6	1.67
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	6	1.67
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD11	10	1.66
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD12	10	1.66
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD13	10	1.66
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD21	10	1.66
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD22	10	1.66
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD23	10	1.66
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD11	10	1.66
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD12	10	1.66
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD13	10	1.66
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD21	10	1.66
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD22	10	1.66
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD23	10	1.66
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	8	1.66
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	6	1.66
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	8	1.66
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	8	1.66
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	8	1.66
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	8	1.66
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	8	1.66
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	8	1.66
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	6	1.66
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	6	1.66
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	6	1.66
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	6	1.65
(1,2495)	1:56:A:SER:H	1:59:A:LEU:HD11	2	1.65
(1,2495)	1:56:A:SER:H	1:59:A:LEU:HD12	2	1.65
(1,2495)	1:56:A:SER:H	1:59:A:LEU:HD13	2	1.65
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	7	1.65
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	6	1.65
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	5	1.65
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	3	1.65
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	5	1.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:174:A:CYS:HB2	1:169:A:GLN:H	2	1.65
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	10	1.65
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	10	1.65
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	10	1.65
(1,329)	1:150:A:ILE:HG21	2:201:A:Z90:HAM	3	1.65
(1,329)	1:150:A:ILE:HG22	2:201:A:Z90:HAM	3	1.65
(1,329)	1:150:A:ILE:HG23	2:201:A:Z90:HAM	3	1.65
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD11	3	1.64
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD12	3	1.64
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD13	3	1.64
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD11	3	1.64
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD12	3	1.64
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD13	3	1.64
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD11	3	1.64
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD12	3	1.64
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD13	3	1.64
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	6	1.64
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD21	4	1.64
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD22	4	1.64
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD23	4	1.64
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD21	4	1.64
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD22	4	1.64
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD23	4	1.64
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD21	4	1.64
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD22	4	1.64
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD23	4	1.64
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	7	1.64
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	7	1.64
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	7	1.64
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD11	9	1.63
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD12	9	1.63
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD13	9	1.63
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	7	1.63
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	7	1.63
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	7	1.63
(1,2492)	1:99:A:GLN:HB2	1:98:A:LEU:H	1	1.63
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	5	1.63
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	5	1.63
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	5	1.63
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	10	1.63
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	10	1.63
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	1	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	1	1.63
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	1	1.63
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	4	1.63
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	4	1.63
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	4	1.63
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	4	1.63
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	4	1.63
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	4	1.63
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	4	1.63
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	4	1.63
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	4	1.63
(1,525)	1:131:A:LEU:HB2	1:183:A:GLU:H	7	1.62
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	2	1.62
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	2	1.62
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	2	1.62
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	2	1.62
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	8	1.62
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	8	1.62
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	8	1.62
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	4	1.62
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	4	1.62
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	4	1.62
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD11	4	1.61
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD12	4	1.61
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD13	4	1.61
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD21	4	1.61
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD22	4	1.61
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD23	4	1.61
(1,1415)	1:34:A:GLU:HA	1:36:A:GLN:H	8	1.61
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	1	1.61
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	1	1.61
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	1	1.61
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	7	1.6
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	6	1.6
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	7	1.6
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	7	1.6
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	9	1.59
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	9	1.59
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	9	1.59
(1,3098)	1:69:A:MET:HG3	1:73:A:MET:H	2	1.59
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	7	1.59
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD11	10	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD12	10	1.59
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD13	10	1.59
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	5	1.59
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	8	1.59
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	7	1.59
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	7	1.59
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	7	1.59
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	3	1.59
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	3	1.59
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	3	1.59
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	10	1.58
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	10	1.58
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	3	1.58
(1,1956)	1:34:A:GLU:HB2	1:36:A:GLN:H	9	1.58
(1,1956)	1:34:A:GLU:HB3	1:36:A:GLN:H	9	1.58
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD11	2	1.58
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD12	2	1.58
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD13	2	1.58
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	7	1.58
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	7	1.58
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	7	1.58
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	6	1.58
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	6	1.58
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	6	1.58
(1,1439)	1:99:A:GLN:HE22	1:95:A:ARG:HG2	5	1.58
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	5	1.58
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	5	1.58
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	5	1.58
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	6	1.58
(1,338)	1:139:A:ARG:HG2	1:49:A:TYR:HE1	2	1.58
(1,338)	1:139:A:ARG:HG2	1:49:A:TYR:HE2	2	1.58
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	9	1.58
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	9	1.58
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	9	1.58
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	10	1.57
(1,2007)	1:69:A:MET:HG2	1:67:A:LEU:H	10	1.57
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE1	6	1.57
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE2	6	1.57
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE3	6	1.57
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	9	1.57
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	9	1.57
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	6	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:31:A:LEU:HB3	1:29:A:ALA:H	7	1.57
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	5	1.57
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	5	1.57
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	5	1.57
(1,1123)	1:94:A:VAL:HB	1:160:A:THR:HB	5	1.56
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	9	1.55
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	9	1.55
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	9	1.55
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	6	1.55
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	6	1.55
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	6	1.55
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	10	1.55
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	7	1.55
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	7	1.55
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	7	1.55
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	8	1.54
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	8	1.54
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	8	1.54
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	2	1.54
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	2	1.54
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	2	1.54
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	9	1.54
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	9	1.54
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	9	1.54
(1,2329)	1:174:A:CYS:H	1:171:A:ASN:H	8	1.54
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	2	1.54
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	6	1.54
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	6	1.54
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	6	1.54
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	6	1.53
(1,3461)	1:132:A:ILE:HG12	1:125:A:ALA:H	3	1.53
(1,2995)	1:176:A:HIS:HA	1:137:A:SER:H	4	1.53
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	1	1.53
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	1	1.53
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	1	1.53
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	5	1.53
(1,2086)	1:93:A:ASN:HD22	1:96:A:GLU:H	2	1.53
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	1	1.53
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	1	1.53
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	1	1.53
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD2	1	1.53
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD3	1	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	4	1.53
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	1	1.53
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	1	1.53
(1,3463)	1:170:A:ARG:HE	1:176:A:HIS:H	1	1.52
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD1	1	1.52
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD2	1	1.52
(1,2492)	1:99:A:GLN:HB2	1:98:A:LEU:H	2	1.52
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	4	1.52
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	10	1.52
(1,1456)	1:160:A:THR:HB	1:158:A:HIS:H	5	1.52
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	8	1.52
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	10	1.52
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	10	1.52
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	10	1.52
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	10	1.52
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	8	1.52
(1,2634)	1:173:A:GLU:HG3	1:172:A:GLU:H	2	1.51
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD1	5	1.51
(1,1776)	1:120:A:PHE:H	1:136:A:TYR:HD2	5	1.51
(1,1530)	1:126:A:GLU:HG3	1:127:A:LYS:H	1	1.51
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD11	5	1.51
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD12	5	1.51
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD13	5	1.51
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG21	8	1.51
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG22	8	1.51
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG23	8	1.51
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	2	1.51
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	2	1.51
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	2	1.51
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	7	1.51
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	7	1.51
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	7	1.51
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	7	1.51
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	7	1.51
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	7	1.51
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	8	1.5
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	8	1.5
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	8	1.5
(1,2503)	1:30:A:GLN:HE22	1:30:A:GLN:H	4	1.5
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	1	1.5
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	5	1.5
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	5	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	5	1.5
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	4	1.5
(1,1116)	1:160:A:THR:HB	1:155:A:GLN:HA	6	1.5
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	2	1.5
(1,3456)	1:158:A:HIS:HD2	1:94:A:VAL:HA	1	1.49
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG11	6	1.49
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG12	6	1.49
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG13	6	1.49
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	8	1.49
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	4	1.49
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	7	1.49
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	1	1.49
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	1	1.49
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	3	1.49
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	3	1.49
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	3	1.49
(1,579)	1:173:A:GLU:HB2	1:171:A:ASN:H	8	1.49
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	1	1.49
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	1	1.49
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	1	1.49
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	8	1.49
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	8	1.49
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	8	1.49
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	4	1.49
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	4	1.49
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	4	1.49
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	5	1.48
(1,2316)	1:171:A:ASN:HB2	1:174:A:CYS:HB3	10	1.48
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	2	1.48
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	2	1.48
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	2	1.48
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	2	1.48
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	2	1.48
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	2	1.48
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	2	1.48
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	2	1.48
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	2	1.48
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	2	1.48
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	2	1.48
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	2	1.48
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	2	1.48
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	2	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	2	1.48
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	7	1.48
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	7	1.48
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	7	1.48
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	8	1.48
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	8	1.48
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	8	1.48
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	1	1.48
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	1	1.48
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	1	1.48
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	1	1.48
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	1	1.48
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZ	1	1.48
(1,294)	2:201:A:Z90:HAT	2:201:A:Z90:HAZA	1	1.48
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	1	1.47
(1,2301)	1:136:A:TYR:HA	1:119:A:SER:H	2	1.47
(1,2125)	1:136:A:TYR:HA	1:119:A:SER:H	2	1.47
(1,2007)	1:69:A:MET:HG2	1:67:A:LEU:H	9	1.47
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	3	1.47
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	3	1.47
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	3	1.47
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	3	1.47
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	5	1.47
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	5	1.47
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	5	1.47
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	10	1.46
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG21	9	1.46
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG22	9	1.46
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG23	9	1.46
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG11	9	1.46
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG12	9	1.46
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG13	9	1.46
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG11	9	1.46
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG12	9	1.46
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG13	9	1.46
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG11	9	1.46
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG12	9	1.46
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG13	9	1.46
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	8	1.46
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE1	2	1.46
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE2	2	1.46
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE3	2	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE1	2	1.46
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE2	2	1.46
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE3	2	1.46
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE1	2	1.46
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE2	2	1.46
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE3	2	1.46
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	4	1.46
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	4	1.46
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	4	1.46
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD1	1	1.46
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD2	1	1.46
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD1	1	1.46
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD2	1	1.46
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD1	1	1.46
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD2	1	1.46
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	8	1.45
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	6	1.45
(1,1930)	1:158:A:HIS:HB2	1:160:A:THR:H	5	1.45
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB1	1	1.45
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB2	1	1.45
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB3	1	1.45
(1,994)	1:165:A:LYS:HE3	1:180:A:LEU:H	4	1.45
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	1	1.45
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	4	1.45
(1,3461)	1:132:A:ILE:HG12	1:125:A:ALA:H	9	1.44
(1,2565)	1:135:A:TYR:HB2	1:179:A:PHE:H	7	1.44
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	6	1.44
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	6	1.44
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	6	1.44
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	1	1.44
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	1	1.44
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	1	1.44
(1,1529)	1:93:A:ASN:HD22	1:93:A:ASN:H	3	1.44
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	3	1.44
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	3	1.44
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	3	1.44
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	3	1.44
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	3	1.44
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	3	1.44
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	3	1.44
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	3	1.44
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	3	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	10	1.44
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	4	1.44
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	9	1.44
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	9	1.44
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	9	1.44
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD11	4	1.44
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD12	4	1.44
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD13	4	1.44
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD11	4	1.44
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD12	4	1.44
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD13	4	1.44
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD11	4	1.44
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD12	4	1.44
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD13	4	1.44
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	6	1.43
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	8	1.43
(1,1738)	1:176:A:HIS:HD2	1:135:A:TYR:H	6	1.43
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB1	6	1.43
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB2	6	1.43
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB3	6	1.43
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	4	1.43
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD21	1	1.43
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD22	1	1.43
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD23	1	1.43
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD21	1	1.43
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD22	1	1.43
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD23	1	1.43
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD21	1	1.43
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD22	1	1.43
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD23	1	1.43
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG21	9	1.43
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG22	9	1.43
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG23	9	1.43
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	10	1.42
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	10	1.42
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	10	1.42
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	3	1.42
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	4	1.42
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	4	1.42
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	4	1.42
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD21	5	1.42
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD22	5	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD23	5	1.42
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD21	5	1.42
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD22	5	1.42
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD23	5	1.42
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD21	5	1.42
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD22	5	1.42
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD23	5	1.42
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	1	1.42
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	2	1.42
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	2	1.42
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	2	1.42
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	10	1.42
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	10	1.42
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	10	1.42
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG21	6	1.42
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG22	6	1.42
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG23	6	1.42
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	2	1.41
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	2	1.41
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	2	1.41
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	9	1.41
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	1	1.41
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	1	1.41
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	1	1.41
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	5	1.41
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	5	1.41
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	5	1.41
(1,2503)	1:30:A:GLN:HE22	1:30:A:GLN:H	5	1.41
(1,2289)	1:158:A:HIS:HB3	1:160:A:THR:H	6	1.41
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	4	1.41
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	9	1.41
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	9	1.41
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	9	1.41
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	7	1.4
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	7	1.4
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	7	1.4
(1,2681)	1:181:A:ILE:HB	1:183:A:GLU:H	9	1.4
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	3	1.4
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	9	1.4
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	5	1.4
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	6	1.4
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	6	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	6	1.4
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	6	1.4
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	7	1.39
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	3	1.39
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	9	1.39
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	9	1.39
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	9	1.39
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	7	1.39
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	7	1.39
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	7	1.39
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	7	1.39
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	7	1.39
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	7	1.39
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	7	1.39
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	7	1.39
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	7	1.39
(1,2479)	1:92:A:SER:HB3	1:93:A:ASN:HD22	7	1.39
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	10	1.39
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	9	1.39
(1,1799)	1:159:A:GLY:H	1:156:A:GLN:H	6	1.39
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD21	10	1.39
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD22	10	1.39
(1,1378)	1:74:A:PHE:HB3	1:11:A:LEU:HD23	10	1.39
(1,1066)	1:139:A:ARG:HG3	1:140:A:GLU:H	7	1.39
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD11	10	1.39
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD12	10	1.39
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD13	10	1.39
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD11	10	1.39
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD12	10	1.39
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD13	10	1.39
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD11	10	1.39
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD12	10	1.39
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD13	10	1.39
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	3	1.39
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	3	1.39
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	3	1.39
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	3	1.38
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	3	1.38
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	3	1.38
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	4	1.38
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	4	1.38
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	4	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3265)	1:92:A:SER:HA	1:157:A:ILE:HD11	7	1.38
(1,3265)	1:92:A:SER:HA	1:157:A:ILE:HD12	7	1.38
(1,3265)	1:92:A:SER:HA	1:157:A:ILE:HD13	7	1.38
(1,3098)	1:69:A:MET:HG3	1:73:A:MET:H	9	1.38
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD21	7	1.38
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD22	7	1.38
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD23	7	1.38
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD21	7	1.38
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD22	7	1.38
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD23	7	1.38
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD21	7	1.38
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD22	7	1.38
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD23	7	1.38
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	3	1.38
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	3	1.38
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	3	1.38
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD11	8	1.38
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD12	8	1.38
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD13	8	1.38
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD21	8	1.38
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD22	8	1.38
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD23	8	1.38
(1,1539)	1:1:A:MET:HE1	1:5:A:VAL:HB	6	1.38
(1,1539)	1:1:A:MET:HE2	1:5:A:VAL:HB	6	1.38
(1,1539)	1:1:A:MET:HE3	1:5:A:VAL:HB	6	1.38
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG11	1	1.38
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG12	1	1.38
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG13	1	1.38
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG11	1	1.38
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG12	1	1.38
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG13	1	1.38
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG11	1	1.38
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG12	1	1.38
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG13	1	1.38
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	4	1.38
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	8	1.38
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	8	1.38
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	8	1.38
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	5	1.37
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	5	1.37
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	5	1.37
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	1	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	1	1.37
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	1	1.37
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	1	1.37
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	1	1.37
(1,1445)	1:137:A:SER:HA	1:139:A:ARG:H	6	1.37
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	7	1.37
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	2	1.37
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	2	1.37
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	2	1.37
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	6	1.37
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	6	1.37
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	6	1.37
(1,3565)	1:131:A:LEU:HG	1:181:A:ILE:H	2	1.36
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	9	1.36
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE1	1	1.36
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE2	1	1.36
(1,1752)	1:43:A:TYR:HE1	1:37:A:PHE:HE1	7	1.36
(1,1752)	1:43:A:TYR:HE1	1:37:A:PHE:HE2	7	1.36
(1,1752)	1:43:A:TYR:HE2	1:37:A:PHE:HE1	7	1.36
(1,1752)	1:43:A:TYR:HE2	1:37:A:PHE:HE2	7	1.36
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD21	7	1.36
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD22	7	1.36
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD23	7	1.36
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG11	3	1.36
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG12	3	1.36
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG13	3	1.36
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG11	3	1.36
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG12	3	1.36
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG13	3	1.36
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG11	3	1.36
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG12	3	1.36
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG13	3	1.36
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD11	9	1.36
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD12	9	1.36
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD13	9	1.36
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD11	9	1.36
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD12	9	1.36
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD13	9	1.36
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD11	9	1.36
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD12	9	1.36
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD13	9	1.36
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	1	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	2	1.35
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	2	1.35
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	2	1.35
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	2	1.35
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	2	1.35
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	2	1.35
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	2	1.35
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	2	1.35
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	2	1.35
(1,1985)	1:136:A:TYR:HD1	1:135:A:TYR:H	2	1.35
(1,1985)	1:136:A:TYR:HD2	1:135:A:TYR:H	2	1.35
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	1	1.35
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG11	8	1.35
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG12	8	1.35
(1,1069)	2:201:A:Z90:HAE	1:5:A:VAL:HG13	8	1.35
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	4	1.35
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	6	1.35
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	1	1.35
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	3	1.35
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	3	1.35
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	3	1.35
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	6	1.35
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	6	1.35
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	6	1.35
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	1	1.35
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	1	1.35
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	1	1.35
(1,195)	1:121:A:ARG:HG2	1:123:A:THR:H	3	1.35
(1,195)	1:121:A:ARG:HG3	1:123:A:THR:H	3	1.35
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	9	1.34
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	9	1.34
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	9	1.34
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	9	1.34
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	7	1.34
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	3	1.34
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	3	1.34
(1,1529)	1:93:A:ASN:HD22	1:93:A:ASN:H	8	1.34
(1,574)	1:120:A:PHE:H	1:121:A:ARG:HB3	3	1.34
(1,120)	1:27:A:LYS:HD2	1:30:A:GLN:H	2	1.34
(1,120)	1:27:A:LYS:HD3	1:30:A:GLN:H	2	1.34
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD11	3	1.34
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD12	3	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD13	3	1.34
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD11	3	1.34
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD12	3	1.34
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD13	3	1.34
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD11	3	1.34
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD12	3	1.34
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD13	3	1.34
(1,3435)	1:146:A:VAL:HB	1:144:A:ASP:H	4	1.33
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	8	1.33
(1,2204)	1:56:A:SER:HB2	1:55:A:ALA:H	10	1.33
(1,1529)	1:93:A:ASN:HD22	1:93:A:ASN:H	7	1.33
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	4	1.33
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	9	1.33
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	8	1.33
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	8	1.33
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	8	1.33
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	6	1.33
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	6	1.33
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	6	1.33
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	3	1.33
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	3	1.33
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	4	1.32
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	4	1.32
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	4	1.32
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	3	1.32
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	3	1.32
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	3	1.32
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	3	1.32
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	3	1.32
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	3	1.32
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	3	1.32
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	3	1.32
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	3	1.32
(1,2634)	1:173:A:GLU:HG3	1:172:A:GLU:H	3	1.32
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	3	1.32
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	3	1.32
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	3	1.32
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	3	1.32
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	3	1.32
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	3	1.32
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	3	1.32
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	3	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	3	1.32
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	9	1.32
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	9	1.32
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	9	1.32
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	8	1.32
(1,2086)	1:93:A:ASN:HD22	1:96:A:GLU:H	10	1.32
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	8	1.32
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	6	1.32
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	6	1.32
(1,998)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	1	1.32
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	8	1.32
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD11	7	1.32
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD12	7	1.32
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD13	7	1.32
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD11	7	1.32
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD12	7	1.32
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD13	7	1.32
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD11	7	1.32
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD12	7	1.32
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD13	7	1.32
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	3	1.31
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	1	1.31
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	3	1.31
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	6	1.31
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	6	1.31
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	6	1.31
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD21	4	1.31
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD22	4	1.31
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD23	4	1.31
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	2	1.31
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	2	1.31
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	2	1.31
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	8	1.31
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	8	1.31
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	8	1.31
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	8	1.31
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	8	1.31
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	8	1.31
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	1	1.31
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	1	1.31
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	1	1.31
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:H	9	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:H	9	1.31
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:H	9	1.31
(1,3457)	1:188:A:GLU:H	1:186:A:SER:HA	2	1.3
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	5	1.3
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	5	1.3
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	5	1.3
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	9	1.3
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	9	1.3
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	9	1.3
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD1	2	1.3
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD2	2	1.3
(1,1271)	1:2:A:TYR:HD1	1:5:A:VAL:H	7	1.3
(1,1271)	1:2:A:TYR:HD2	1:5:A:VAL:H	7	1.3
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	6	1.3
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	6	1.3
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	6	1.3
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	6	1.3
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	7	1.29
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	7	1.29
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	7	1.29
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	2	1.29
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	2	1.29
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	2	1.29
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD21	3	1.29
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD22	3	1.29
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD23	3	1.29
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	4	1.29
(1,1066)	1:139:A:ARG:HG3	1:140:A:GLU:H	1	1.29
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	7	1.29
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	6	1.29
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	10	1.29
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	10	1.29
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	10	1.29
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	7	1.29
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	7	1.29
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	7	1.29
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	8	1.29
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	6	1.28
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	6	1.28
(1,2788)	1:10:A:GLU:HG2	1:22:A:TRP:HE1	9	1.28
(1,2492)	1:99:A:GLN:HB2	1:98:A:LEU:H	3	1.28
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	6	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	6	1.28
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	6	1.28
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	7	1.28
(1,1725)	1:128:A:GLY:H	1:130:A:GLY:H	6	1.28
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE1	3	1.28
(1,1458)	2:201:A:Z90:HAJ	1:112:A:TYR:HE2	3	1.28
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	9	1.28
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	9	1.28
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	9	1.28
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	6	1.28
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	6	1.28
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	6	1.28
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	8	1.28
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	8	1.28
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	8	1.28
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	1	1.28
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	1	1.28
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	1	1.28
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	10	1.28
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	3	1.28
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	3	1.28
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	3	1.28
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	3	1.28
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	3	1.28
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	3	1.28
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	9	1.28
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	9	1.28
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	4	1.27
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	10	1.27
(1,2927)	1:76:A:VAL:H	1:152:A:THR:HG21	8	1.27
(1,2927)	1:76:A:VAL:H	1:152:A:THR:HG22	8	1.27
(1,2927)	1:76:A:VAL:H	1:152:A:THR:HG23	8	1.27
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	6	1.27
(1,2266)	1:171:A:ASN:HD22	1:173:A:GLU:H	8	1.27
(1,2007)	1:69:A:MET:HG2	1:67:A:LEU:H	2	1.27
(1,1935)	1:135:A:TYR:HD1	1:119:A:SER:H	9	1.27
(1,1935)	1:135:A:TYR:HD2	1:119:A:SER:H	9	1.27
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD21	8	1.27
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD22	8	1.27
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD23	8	1.27
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	4	1.27
(1,1565)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	1	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1187)	1:31:A:LEU:HA	1:35:A:GLY:H	9	1.27
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	7	1.27
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	7	1.27
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	7	1.27
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	4	1.27
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	7	1.27
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	7	1.27
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	7	1.27
(1,96)	1:180:A:LEU:HG	1:131:A:LEU:H	8	1.27
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD11	6	1.26
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD12	6	1.26
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD13	6	1.26
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	8	1.26
(1,2995)	1:176:A:HIS:HA	1:137:A:SER:H	7	1.26
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	10	1.26
(1,2212)	1:184:A:LYS:HD2	1:184:A:LYS:H	9	1.26
(1,2212)	1:184:A:LYS:HD3	1:184:A:LYS:H	9	1.26
(1,1935)	1:135:A:TYR:HD1	1:119:A:SER:H	10	1.26
(1,1935)	1:135:A:TYR:HD2	1:119:A:SER:H	10	1.26
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	8	1.26
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	8	1.26
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	8	1.26
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	10	1.26
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	1	1.26
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	1	1.26
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	1	1.26
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG21	3	1.26
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG22	3	1.26
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG23	3	1.26
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	7	1.26
(1,3461)	1:132:A:ILE:HG12	1:125:A:ALA:H	7	1.25
(1,3232)	1:32:A:ASP:HB3	1:27:A:LYS:H	9	1.25
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	1	1.25
(1,2086)	1:93:A:ASN:HD22	1:96:A:GLU:H	7	1.25
(1,2009)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	9	1.25
(1,2009)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	9	1.25
(1,2009)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	9	1.25
(1,2007)	1:69:A:MET:HG2	1:67:A:LEU:H	7	1.25
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	8	1.25
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	10	1.25
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	10	1.25
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	10	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	2	1.25
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	4	1.25
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	4	1.25
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	4	1.25
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	4	1.25
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	4	1.25
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	4	1.25
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	4	1.25
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	4	1.25
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	4	1.25
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	4	1.25
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	4	1.25
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	4	1.25
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD2	10	1.25
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD3	10	1.25
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	9	1.25
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	2	1.25
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	2	1.25
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	2	1.25
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	10	1.25
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	10	1.25
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	10	1.25
(1,245)	1:66:A:ILE:HB	1:68:A:GLN:H	7	1.25
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	6	1.25
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	6	1.25
(2,4)	1:139:A:ARG:HH21	2:201:A:Z90:OAB	8	1.24
(1,3384)	1:120:A:PHE:HD1	1:135:A:TYR:H	1	1.24
(1,3384)	1:120:A:PHE:HD2	1:135:A:TYR:H	1	1.24
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	1	1.24
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	1	1.24
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	1	1.24
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	8	1.24
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	8	1.24
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	8	1.24
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	1	1.24
(1,2116)	1:161:A:GLU:HG3	1:160:A:THR:HA	7	1.24
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	1	1.24
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	5	1.24
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	5	1.24
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	5	1.24
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	4	1.24
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	4	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	4	1.24
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	7	1.24
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	2	1.24
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	7	1.23
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	3	1.23
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	4	1.23
(1,2116)	1:161:A:GLU:HG3	1:160:A:THR:HA	5	1.23
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	8	1.23
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	8	1.23
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	8	1.23
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	5	1.23
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	5	1.23
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	5	1.23
(1,909)	1:65:A:GLU:HG2	1:64:A:GLY:H	9	1.23
(1,909)	1:65:A:GLU:HG3	1:64:A:GLY:H	9	1.23
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	6	1.23
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	6	1.23
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	6	1.23
(1,3098)	1:69:A:MET:HG3	1:73:A:MET:H	6	1.22
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	9	1.22
(1,2795)	1:16:A:ASN:HD22	1:16:A:ASN:H	5	1.22
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	3	1.22
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	4	1.22
(1,1066)	1:139:A:ARG:HG3	1:140:A:GLU:H	6	1.22
(1,524)	1:124:A:ASP:HB2	1:131:A:LEU:H	9	1.22
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	7	1.22
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	7	1.22
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	5	1.21
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG11	8	1.21
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG12	8	1.21
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG13	8	1.21
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB1	2	1.21
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB2	2	1.21
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB3	2	1.21
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	7	1.21
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	7	1.21
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	7	1.21
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	4	1.21
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	4	1.21
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	4	1.21
(1,2266)	1:171:A:ASN:HD22	1:173:A:GLU:H	1	1.21
(1,2204)	1:56:A:SER:HB2	1:55:A:ALA:H	6	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	7	1.21
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	7	1.21
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	7	1.21
(1,1913)	1:59:A:LEU:HD11	1:66:A:ILE:HG21	2	1.21
(1,1913)	1:59:A:LEU:HD11	1:66:A:ILE:HG22	2	1.21
(1,1913)	1:59:A:LEU:HD11	1:66:A:ILE:HG23	2	1.21
(1,1913)	1:59:A:LEU:HD12	1:66:A:ILE:HG21	2	1.21
(1,1913)	1:59:A:LEU:HD12	1:66:A:ILE:HG22	2	1.21
(1,1913)	1:59:A:LEU:HD12	1:66:A:ILE:HG23	2	1.21
(1,1913)	1:59:A:LEU:HD13	1:66:A:ILE:HG21	2	1.21
(1,1913)	1:59:A:LEU:HD13	1:66:A:ILE:HG22	2	1.21
(1,1913)	1:59:A:LEU:HD13	1:66:A:ILE:HG23	2	1.21
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	9	1.21
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	5	1.21
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	5	1.21
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	5	1.21
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	10	1.21
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	10	1.21
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	10	1.21
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	1	1.21
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	1	1.21
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	1	1.21
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	2	1.21
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	2	1.21
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	2	1.21
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	2	1.21
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	2	1.21
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	2	1.21
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	2	1.21
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	2	1.21
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	2	1.21
(1,3353)	1:91:A:GLY:H	1:93:A:ASN:H	7	1.2
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	10	1.2
(1,2967)	1:160:A:THR:H	1:157:A:ILE:H	6	1.2
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	3	1.2
(1,1985)	1:136:A:TYR:HD1	1:135:A:TYR:H	7	1.2
(1,1985)	1:136:A:TYR:HD2	1:135:A:TYR:H	7	1.2
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	1	1.2
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	2	1.2
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD11	6	1.2
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD12	6	1.2
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD13	6	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD21	6	1.2
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD22	6	1.2
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD23	6	1.2
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	2	1.2
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	1	1.2
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	1	1.2
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	1	1.2
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	1	1.2
(1,935)	1:125:A:ALA:HA	1:132:A:ILE:HB	3	1.2
(1,626)	1:177:A:THR:HB	1:170:A:ARG:H	7	1.2
(1,558)	1:125:A:ALA:HA	1:132:A:ILE:HG13	6	1.2
(1,316)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	3	1.2
(1,316)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	3	1.2
(1,316)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	3	1.2
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	8	1.2
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	8	1.2
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	8	1.2
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	7	1.2
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	7	1.2
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	7	1.2
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	10	1.2
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	10	1.2
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB2	7	1.2
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB3	7	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	6	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	6	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	6	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	6	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	6	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	6	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	6	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	6	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	6	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	9	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	9	1.2
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	9	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	9	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	9	1.2
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	9	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	9	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	9	1.2
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	9	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3563)	1:131:A:LEU:HB3	1:181:A:ILE:H	7	1.19
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	6	1.19
(1,2503)	1:30:A:GLN:HE22	1:30:A:GLN:H	2	1.19
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	9	1.19
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	9	1.19
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	9	1.19
(1,1738)	1:176:A:HIS:HD2	1:135:A:TYR:H	4	1.19
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	9	1.19
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	4	1.19
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	4	1.19
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	4	1.19
(1,909)	1:65:A:GLU:HG2	1:64:A:GLY:H	6	1.19
(1,909)	1:65:A:GLU:HG3	1:64:A:GLY:H	6	1.19
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	1	1.19
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	1	1.19
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	1	1.19
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	9	1.19
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	9	1.19
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	9	1.19
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	6	1.19
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	6	1.19
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	6	1.19
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD1	3	1.19
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD2	3	1.19
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD1	3	1.19
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD2	3	1.19
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD1	3	1.19
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD2	3	1.19
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	3	1.18
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	4	1.18
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG11	5	1.18
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG12	5	1.18
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG13	5	1.18
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG11	10	1.18
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG12	10	1.18
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG13	10	1.18
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	5	1.18
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD11	2	1.18
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD12	2	1.18
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD13	2	1.18
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD11	2	1.18
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD12	2	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD13	2	1.18
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD11	2	1.18
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD12	2	1.18
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD13	2	1.18
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	9	1.18
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	10	1.18
(1,982)	1:21:A:VAL:HG11	1:20:A:GLU:H	3	1.18
(1,982)	1:21:A:VAL:HG12	1:20:A:GLU:H	3	1.18
(1,982)	1:21:A:VAL:HG13	1:20:A:GLU:H	3	1.18
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	6	1.18
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	2	1.18
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	2	1.18
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	2	1.18
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	4	1.18
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	4	1.18
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	4	1.18
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	4	1.18
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	4	1.18
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	4	1.18
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	2	1.17
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	2	1.17
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	10	1.17
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	10	1.17
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	8	1.17
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD21	9	1.17
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD22	9	1.17
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD23	9	1.17
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	5	1.17
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD2	3	1.17
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD3	3	1.17
(1,1321)	1:49:A:TYR:HE1	1:49:A:TYR:H	2	1.17
(1,1321)	1:49:A:TYR:HE2	1:49:A:TYR:H	2	1.17
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	9	1.17
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG11	3	1.17
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG12	3	1.17
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG13	3	1.17
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG11	3	1.17
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG12	3	1.17
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG13	3	1.17
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG11	3	1.17
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG12	3	1.17
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG13	3	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	3	1.17
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	3	1.17
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	3	1.17
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	5	1.17
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	5	1.17
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	5	1.17
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	10	1.16
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	10	1.16
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	10	1.16
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	9	1.16
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	9	1.16
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	9	1.16
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	1	1.16
(1,1810)	1:93:A:ASN:HD22	1:96:A:GLU:HB3	8	1.16
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	6	1.16
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	7	1.16
(1,1019)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	1	1.16
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD11	2	1.16
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD12	2	1.16
(1,597)	1:27:A:LYS:H	1:51:A:LEU:HD13	2	1.16
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	8	1.16
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	7	1.16
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	7	1.16
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	7	1.16
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	2	1.15
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	10	1.15
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	10	1.15
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	10	1.15
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	3	1.15
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	10	1.15
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	1	1.15
(1,2634)	1:173:A:GLU:HG3	1:172:A:GLU:H	4	1.15
(1,2513)	1:142:A:LEU:HD21	1:139:A:ARG:H	3	1.15
(1,2513)	1:142:A:LEU:HD22	1:139:A:ARG:H	3	1.15
(1,2513)	1:142:A:LEU:HD23	1:139:A:ARG:H	3	1.15
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	6	1.15
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	6	1.15
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	9	1.15
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	9	1.15
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	9	1.15
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	7	1.15
(1,289)	1:149:A:ILE:HG21	2:201:A:Z90:HAI	9	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:149:A:ILE:HG22	2:201:A:Z90:HAI	9	1.15
(1,289)	1:149:A:ILE:HG23	2:201:A:Z90:HAI	9	1.15
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	5	1.14
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	2	1.14
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	1	1.14
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	1	1.14
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	1	1.14
(1,2453)	2:201:A:Z90:HAM	1:90:A:LEU:HD11	9	1.14
(1,2453)	2:201:A:Z90:HAM	1:90:A:LEU:HD12	9	1.14
(1,2453)	2:201:A:Z90:HAM	1:90:A:LEU:HD13	9	1.14
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	1	1.14
(1,2086)	1:93:A:ASN:HD22	1:96:A:GLU:H	5	1.14
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	9	1.14
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	1	1.14
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	1	1.14
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD21	5	1.14
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD22	5	1.14
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD23	5	1.14
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	1	1.14
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	1	1.14
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	1	1.14
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD11	8	1.14
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD12	8	1.14
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD13	8	1.14
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD21	8	1.14
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD22	8	1.14
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD23	8	1.14
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	2	1.14
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	9	1.14
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	5	1.14
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	5	1.14
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	5	1.14
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	5	1.14
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	5	1.14
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	5	1.14
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	5	1.14
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	5	1.14
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	5	1.14
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	5	1.14
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	5	1.14
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	5	1.14
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	5	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	5	1.14
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	5	1.14
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	7	1.14
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	7	1.14
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	7	1.14
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	5	1.14
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	5	1.14
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	5	1.13
(1,3098)	1:69:A:MET:HG3	1:73:A:MET:H	10	1.13
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	8	1.13
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	2	1.13
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	2	1.13
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	2	1.13
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	1	1.13
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	2	1.13
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	9	1.13
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG11	7	1.13
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG12	7	1.13
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG13	7	1.13
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG11	7	1.13
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG12	7	1.13
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG13	7	1.13
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG11	7	1.13
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG12	7	1.13
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG13	7	1.13
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD11	9	1.13
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD12	9	1.13
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD13	9	1.13
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD21	9	1.13
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD22	9	1.13
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD23	9	1.13
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD11	4	1.13
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD12	4	1.13
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD13	4	1.13
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	5	1.13
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	5	1.13
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	5	1.13
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	1	1.13
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	1	1.13
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	1	1.13
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG11	6	1.13
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG12	6	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:54:A:ALA:HB1	1:58:A:VAL:HG13	6	1.13
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG11	6	1.13
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG12	6	1.13
(1,970)	1:54:A:ALA:HB2	1:58:A:VAL:HG13	6	1.13
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG11	6	1.13
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG12	6	1.13
(1,970)	1:54:A:ALA:HB3	1:58:A:VAL:HG13	6	1.13
(1,316)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	6	1.13
(1,316)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	6	1.13
(1,316)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	6	1.13
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	7	1.13
(1,245)	1:66:A:ILE:HB	1:68:A:GLN:H	6	1.13
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD21	3	1.12
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD22	3	1.12
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD23	3	1.12
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD21	3	1.12
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD22	3	1.12
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD23	3	1.12
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD21	3	1.12
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD22	3	1.12
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD23	3	1.12
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	8	1.12
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	8	1.12
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	8	1.12
(1,3107)	1:24:A:ASP:HB3	1:22:A:TRP:H	10	1.12
(1,3046)	1:11:A:LEU:HB2	1:13:A:VAL:H	5	1.12
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	5	1.12
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	5	1.12
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	5	1.12
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	7	1.12
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	7	1.12
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	7	1.12
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG11	3	1.12
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG12	3	1.12
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG13	3	1.12
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	8	1.12
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	8	1.12
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	8	1.12
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	8	1.12
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	8	1.12
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	8	1.12
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	8	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	8	1.12
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	8	1.12
(1,2340)	1:139:A:ARG:HG2	1:141:A:GLY:H	8	1.12
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	9	1.12
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	2	1.12
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	2	1.12
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	2	1.12
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	4	1.12
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD2	4	1.12
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD3	4	1.12
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD11	6	1.12
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD12	6	1.12
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD13	6	1.12
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD11	6	1.12
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD12	6	1.12
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD13	6	1.12
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD11	6	1.12
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD12	6	1.12
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD13	6	1.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD21	6	1.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD22	6	1.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD23	6	1.12
(1,563)	1:174:A:CYS:H	1:171:A:ASN:H	8	1.12
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	2	1.12
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	2	1.12
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	2	1.12
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	2	1.12
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:H	2	1.12
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:H	2	1.12
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:H	2	1.12
(1,2469)	1:11:A:LEU:HB2	1:13:A:VAL:H	5	1.11
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	1	1.11
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	1	1.11
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	1	1.11
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	2	1.11
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	4	1.11
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	5	1.11
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	4	1.11
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	10	1.11
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG21	8	1.11
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG22	8	1.11
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG23	8	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD21	9	1.11
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD22	9	1.11
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD23	9	1.11
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG11	5	1.11
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG12	5	1.11
(1,1414)	1:149:A:ILE:HD11	1:153:A:VAL:HG13	5	1.11
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG11	5	1.11
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG12	5	1.11
(1,1414)	1:149:A:ILE:HD12	1:153:A:VAL:HG13	5	1.11
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG11	5	1.11
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG12	5	1.11
(1,1414)	1:149:A:ILE:HD13	1:153:A:VAL:HG13	5	1.11
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	1	1.11
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	8	1.11
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	8	1.11
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	8	1.11
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	1	1.11
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	9	1.11
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	5	1.11
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	8	1.11
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	8	1.11
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	8	1.11
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	8	1.11
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	8	1.11
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	8	1.11
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG21	4	1.1
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG22	4	1.1
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG23	4	1.1
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	5	1.1
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	5	1.1
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	5	1.1
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD21	7	1.1
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD22	7	1.1
(1,2523)	1:55:A:ALA:H	1:51:A:LEU:HD23	7	1.1
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	9	1.1
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	9	1.1
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	10	1.1
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	10	1.1
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	10	1.1
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD1	10	1.1
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD2	10	1.1
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD11	9	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD12	9	1.1
(1,752)	1:98:A:LEU:HD21	1:147:A:ILE:HD13	9	1.1
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD11	9	1.1
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD12	9	1.1
(1,752)	1:98:A:LEU:HD22	1:147:A:ILE:HD13	9	1.1
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD11	9	1.1
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD12	9	1.1
(1,752)	1:98:A:LEU:HD23	1:147:A:ILE:HD13	9	1.1
(1,522)	1:96:A:GLU:HG2	1:93:A:ASN:H	9	1.1
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	10	1.1
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	10	1.1
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	10	1.1
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD21	4	1.09
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD22	4	1.09
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD23	4	1.09
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	6	1.09
(1,3107)	1:24:A:ASP:HB3	1:22:A:TRP:H	5	1.09
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	6	1.09
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	6	1.09
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	6	1.09
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	7	1.09
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG11	4	1.09
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG12	4	1.09
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG13	4	1.09
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	7	1.09
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	4	1.09
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	4	1.09
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	4	1.09
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	8	1.09
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	8	1.09
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	8	1.09
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	8	1.09
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	8	1.09
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	3	1.09
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	10	1.09
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	9	1.09
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG21	1	1.09
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG22	1	1.09
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG23	1	1.09
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	5	1.09
(1,666)	1:27:A:LYS:HD3	1:33:A:GLU:H	7	1.09
(1,3467)	1:2:A:TYR:HA	1:43:A:TYR:H	7	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	6	1.08
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	8	1.08
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	8	1.08
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	8	1.08
(1,2863)	1:126:A:GLU:H	1:130:A:GLY:H	1	1.08
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG11	6	1.08
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG12	6	1.08
(1,2828)	1:38:A:LEU:HA	1:39:A:VAL:HG13	6	1.08
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	5	1.08
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	5	1.08
(1,2196)	1:164:A:MET:HA	1:165:A:LYS:HD2	2	1.08
(1,1927)	1:120:A:PHE:HE1	1:119:A:SER:H	9	1.08
(1,1927)	1:120:A:PHE:HE2	1:119:A:SER:H	9	1.08
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	5	1.08
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	3	1.08
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	10	1.08
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD1	1	1.08
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD2	1	1.08
(1,1026)	1:56:A:SER:HG	1:61:A:LEU:H	1	1.08
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	2	1.08
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	2	1.08
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	2	1.08
(1,624)	1:92:A:SER:H	1:96:A:GLU:HG3	2	1.08
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	9	1.08
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	9	1.08
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	9	1.08
(1,265)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	3	1.08
(1,265)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	3	1.08
(1,265)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	3	1.08
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	2	1.08
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	2	1.08
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	2	1.08
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB1	8	1.08
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB2	8	1.08
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB3	8	1.08
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB1	8	1.08
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB2	8	1.08
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB3	8	1.08
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB1	8	1.08
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB2	8	1.08
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB3	8	1.08
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB1	8	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB2	8	1.08
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB3	8	1.08
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB1	8	1.08
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB2	8	1.08
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB3	8	1.08
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB1	8	1.08
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB2	8	1.08
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB3	8	1.08
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	6	1.07
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD1	5	1.07
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD2	5	1.07
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD1	5	1.07
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD2	5	1.07
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD1	5	1.07
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD2	5	1.07
(1,2410)	1:57:A:LYS:H	1:59:A:LEU:HD11	2	1.07
(1,2410)	1:57:A:LYS:H	1:59:A:LEU:HD12	2	1.07
(1,2410)	1:57:A:LYS:H	1:59:A:LEU:HD13	2	1.07
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	10	1.07
(1,2196)	1:164:A:MET:HA	1:165:A:LYS:HD2	1	1.07
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	1	1.07
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	8	1.07
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	4	1.07
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	4	1.07
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	4	1.07
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG21	5	1.06
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG22	5	1.06
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG23	5	1.06
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG21	5	1.06
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG22	5	1.06
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG23	5	1.06
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG21	5	1.06
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG22	5	1.06
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG23	5	1.06
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	2	1.06
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG11	3	1.06
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG12	3	1.06
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG13	3	1.06
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG11	3	1.06
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG12	3	1.06
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG13	3	1.06
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	8	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	4	1.06
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	9	1.06
(1,1396)	1:158:A:HIS:HD2	1:154:A:ALA:HA	2	1.06
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	10	1.06
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	3	1.06
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG21	4	1.06
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG22	4	1.06
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG23	4	1.06
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	1	1.05
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	1	1.05
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	1	1.05
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	6	1.05
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	6	1.05
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	6	1.05
(1,2795)	1:16:A:ASN:HD22	1:16:A:ASN:H	3	1.05
(1,2552)	1:99:A:GLN:HE22	1:96:A:GLU:H	8	1.05
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	5	1.05
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	1	1.05
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	2	1.05
(1,1808)	1:9:A:LEU:H	1:5:A:VAL:H	7	1.05
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	9	1.05
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	9	1.05
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	9	1.05
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	6	1.05
(1,548)	1:143:A:GLN:HE22	1:144:A:ASP:H	8	1.05
(1,3297)	1:143:A:GLN:HE22	1:142:A:LEU:H	4	1.04
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	6	1.04
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	1	1.04
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	1	1.04
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	1	1.04
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	3	1.04
(1,2007)	1:69:A:MET:HG2	1:67:A:LEU:H	6	1.04
(1,1810)	1:93:A:ASN:HD22	1:96:A:GLU:HB3	3	1.04
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	6	1.04
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	2	1.04
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	3	1.04
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	7	1.04
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD11	6	1.04
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD12	6	1.04
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD13	6	1.04
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD21	6	1.04
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD22	6	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:183:A:GLU:H	1:131:A:LEU:HD23	6	1.04
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG21	3	1.04
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG22	3	1.04
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG23	3	1.04
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG21	3	1.04
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG22	3	1.04
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG23	3	1.04
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG21	3	1.04
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG22	3	1.04
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG23	3	1.04
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	2	1.04
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	8	1.04
(1,548)	1:143:A:GLN:HE22	1:144:A:ASP:H	2	1.04
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	3	1.04
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	3	1.04
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	3	1.04
(1,3565)	1:131:A:LEU:HG	1:181:A:ILE:H	5	1.03
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG21	6	1.03
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG22	6	1.03
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG23	6	1.03
(1,3393)	1:155:A:GLN:HB2	1:159:A:GLY:H	6	1.03
(1,3393)	1:155:A:GLN:HB3	1:159:A:GLY:H	6	1.03
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD21	1	1.03
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD22	1	1.03
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD23	1	1.03
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	5	1.03
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	5	1.03
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	5	1.03
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	8	1.03
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	1	1.03
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	1	1.03
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	1	1.03
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	10	1.03
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD21	7	1.03
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD22	7	1.03
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD23	7	1.03
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	2	1.03
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	3	1.03
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	5	1.03
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	10	1.03
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	10	1.03
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	10	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	10	1.03
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	8	1.03
(1,1123)	1:94:A:VAL:HB	1:160:A:THR:HB	6	1.03
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	1	1.03
(1,401)	1:132:A:ILE:HA	1:125:A:ALA:H	9	1.03
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	4	1.03
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	4	1.03
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	4	1.03
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	10	1.03
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	10	1.03
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	7	1.03
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	7	1.03
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	7	1.03
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	9	1.03
(1,40)	1:57:A:LYS:HB2	1:58:A:VAL:HG11	6	1.03
(1,40)	1:57:A:LYS:HB2	1:58:A:VAL:HG12	6	1.03
(1,40)	1:57:A:LYS:HB2	1:58:A:VAL:HG13	6	1.03
(1,40)	1:57:A:LYS:HB3	1:58:A:VAL:HG11	6	1.03
(1,40)	1:57:A:LYS:HB3	1:58:A:VAL:HG12	6	1.03
(1,40)	1:57:A:LYS:HB3	1:58:A:VAL:HG13	6	1.03
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	9	1.02
(1,3354)	1:27:A:LYS:HD3	1:28:A:GLU:H	9	1.02
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	2	1.02
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	2	1.02
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	7	1.02
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	7	1.02
(1,1876)	1:10:A:GLU:HG3	1:22:A:TRP:HE1	9	1.02
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	1	1.02
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	10	1.02
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	6	1.02
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	6	1.02
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	6	1.02
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	1	1.02
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	8	1.02
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	8	1.02
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	8	1.02
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	10	1.02
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	10	1.02
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	10	1.02
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	9	1.02
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	9	1.02
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	8	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	8	1.02
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	7	1.01
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	3	1.01
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	1	1.01
(1,2805)	1:26:A:LYS:HE3	1:22:A:TRP:HE1	9	1.01
(1,2786)	1:14:A:ILE:HG13	1:22:A:TRP:HE1	7	1.01
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG11	1	1.01
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG12	1	1.01
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG13	1	1.01
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG11	1	1.01
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG12	1	1.01
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG13	1	1.01
(1,2266)	1:171:A:ASN:HD22	1:173:A:GLU:H	7	1.01
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	2	1.01
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	8	1.01
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	1	1.01
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	1	1.01
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	1	1.01
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD21	4	1.01
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD22	4	1.01
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD23	4	1.01
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD21	4	1.01
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD22	4	1.01
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD23	4	1.01
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD21	4	1.01
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD22	4	1.01
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD23	4	1.01
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	5	1.01
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	9	1.01
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	9	1.01
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	9	1.01
(1,265)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	6	1.01
(1,265)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	6	1.01
(1,265)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	6	1.01
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	10	1.01
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	10	1.01
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	9	1.0
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	4	1.0
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	4	1.0
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	4	1.0
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	2	1.0
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	5	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1495)	1:125:A:ALA:HB1	1:131:A:LEU:H	1	1.0
(1,1495)	1:125:A:ALA:HB2	1:131:A:LEU:H	1	1.0
(1,1495)	1:125:A:ALA:HB3	1:131:A:LEU:H	1	1.0
(1,1187)	1:31:A:LEU:HA	1:35:A:GLY:H	1	1.0
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	5	1.0
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	7	1.0
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	6	1.0
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	6	1.0
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	6	1.0
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD11	10	1.0
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD12	10	1.0
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD13	10	1.0
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	5	1.0
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	5	1.0
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	5	1.0
(1,245)	1:66:A:ILE:HB	1:68:A:GLN:H	10	1.0
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	10	0.99
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	8	0.99
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	1	0.99
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	2	0.99
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	7	0.99
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	3	0.99
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	3	0.99
(1,1615)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	3	0.99
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	10	0.99
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	4	0.99
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	4	0.99
(1,1520)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	4	0.99
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	7	0.99
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD11	2	0.99
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD12	2	0.99
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD13	2	0.99
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	1	0.99
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG11	3	0.99
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG12	3	0.99
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG13	3	0.99
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	7	0.99
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	6	0.99
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG21	6	0.99
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG22	6	0.99
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG23	6	0.99
(1,574)	1:120:A:PHE:H	1:121:A:ARG:HB3	1	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	4	0.99
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	4	0.99
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	4	0.99
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	2	0.99
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	2	0.99
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	2	0.99
(1,245)	1:69:A:MET:HE1	1:68:A:GLN:H	2	0.99
(1,245)	1:69:A:MET:HE2	1:68:A:GLN:H	2	0.99
(1,245)	1:69:A:MET:HE3	1:68:A:GLN:H	2	0.99
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	1	0.99
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	1	0.99
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	5	0.98
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	8	0.98
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	9	0.98
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	8	0.98
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	10	0.98
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	10	0.98
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	10	0.98
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	9	0.98
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	3	0.98
(1,1951)	1:184:A:LYS:HE3	1:184:A:LYS:HA	2	0.98
(1,1701)	1:95:A:ARG:HG3	1:94:A:VAL:HG11	8	0.98
(1,1701)	1:95:A:ARG:HG3	1:94:A:VAL:HG12	8	0.98
(1,1701)	1:95:A:ARG:HG3	1:94:A:VAL:HG13	8	0.98
(1,1633)	1:146:A:VAL:HB	1:149:A:ILE:HD11	10	0.98
(1,1633)	1:146:A:VAL:HB	1:149:A:ILE:HD12	10	0.98
(1,1633)	1:146:A:VAL:HB	1:149:A:ILE:HD13	10	0.98
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	3	0.98
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG11	5	0.98
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG12	5	0.98
(1,1178)	1:152:A:THR:H	1:153:A:VAL:HG13	5	0.98
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	6	0.98
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	6	0.98
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	6	0.98
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	9	0.98
(1,624)	1:92:A:SER:H	1:96:A:GLU:HG3	6	0.98
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAY	5	0.98
(1,295)	2:201:A:Z90:HAT	2:201:A:Z90:HAYA	5	0.98
(1,245)	1:69:A:MET:HE1	1:68:A:GLN:H	1	0.98
(1,245)	1:69:A:MET:HE2	1:68:A:GLN:H	1	0.98
(1,245)	1:69:A:MET:HE3	1:68:A:GLN:H	1	0.98
(1,122)	1:27:A:LYS:HD2	1:31:A:LEU:H	4	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:27:A:LYS:HD3	1:31:A:LEU:H	4	0.98
(1,2552)	1:99:A:GLN:HE22	1:96:A:GLU:H	9	0.97
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	2	0.97
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	2	0.97
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	2	0.97
(1,1368)	1:183:A:GLU:HG2	1:163:A:ASP:H	4	0.97
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	8	0.97
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	7	0.97
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	1	0.97
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	2	0.97
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	9	0.97
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	9	0.97
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	9	0.97
(1,245)	1:66:A:ILE:HB	1:68:A:GLN:H	5	0.97
(2,4)	1:139:A:ARG:HH21	2:201:A:Z90:OAB	4	0.96
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	6	0.96
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	9	0.96
(1,3234)	1:100:A:ASN:HD22	1:96:A:GLU:HB3	9	0.96
(1,2720)	1:140:A:GLU:HG2	1:142:A:LEU:H	9	0.96
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	10	0.96
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	10	0.96
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	10	0.96
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	5	0.96
(1,2503)	1:30:A:GLN:HE22	1:30:A:GLN:H	10	0.96
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	9	0.96
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	9	0.96
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	9	0.96
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	7	0.96
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	3	0.96
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	7	0.96
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	5	0.96
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	2	0.96
(1,1123)	1:94:A:VAL:HB	1:160:A:THR:HB	7	0.96
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	3	0.96
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	3	0.96
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	3	0.96
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	10	0.96
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	6	0.96
(1,574)	1:120:A:PHE:H	1:121:A:ARG:HB3	8	0.96
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	3	0.96
(1,525)	1:131:A:LEU:HB2	1:183:A:GLU:H	9	0.96
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG11	3	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG12	3	0.96
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG13	3	0.96
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG11	6	0.96
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG12	6	0.96
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG13	6	0.96
(1,335)	1:101:A:LEU:HD11	2:201:A:Z90:HAH	7	0.96
(1,335)	1:101:A:LEU:HD12	2:201:A:Z90:HAH	7	0.96
(1,335)	1:101:A:LEU:HD13	2:201:A:Z90:HAH	7	0.96
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	4	0.96
(1,245)	1:69:A:MET:HE1	1:68:A:GLN:H	4	0.96
(1,245)	1:69:A:MET:HE2	1:68:A:GLN:H	4	0.96
(1,245)	1:69:A:MET:HE3	1:68:A:GLN:H	4	0.96
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD1	7	0.95
(1,3323)	1:137:A:SER:H	1:120:A:PHE:HD2	7	0.95
(1,2896)	1:136:A:TYR:H	1:119:A:SER:H	7	0.95
(1,2871)	1:181:A:ILE:H	1:130:A:GLY:H	2	0.95
(1,2717)	1:49:A:TYR:HB3	1:46:A:SER:H	2	0.95
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	7	0.95
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	9	0.95
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	9	0.95
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	9	0.95
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG21	6	0.95
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG22	6	0.95
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG23	6	0.95
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	9	0.95
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE1	2	0.95
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE2	2	0.95
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	7	0.95
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	6	0.95
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD11	2	0.95
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD12	2	0.95
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD13	2	0.95
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	9	0.95
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	8	0.95
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	8	0.95
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	8	0.95
(1,195)	1:121:A:ARG:HG2	1:123:A:THR:H	8	0.95
(1,195)	1:121:A:ARG:HG3	1:123:A:THR:H	8	0.95
(2,1)	1:135:A:TYR:HH	2:201:A:Z90:OAC	6	0.94
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD11	4	0.94
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD12	4	0.94
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD13	4	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD11	4	0.94
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD12	4	0.94
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD13	4	0.94
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD11	4	0.94
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD12	4	0.94
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD13	4	0.94
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	3	0.94
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	3	0.94
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	3	0.94
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	2	0.94
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	2	0.94
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	2	0.94
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	5	0.94
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	8	0.94
(1,2634)	1:173:A:GLU:HG3	1:172:A:GLU:H	8	0.94
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG11	7	0.94
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG12	7	0.94
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG13	7	0.94
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG11	7	0.94
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG12	7	0.94
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG13	7	0.94
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG11	7	0.94
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG12	7	0.94
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG13	7	0.94
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	9	0.94
(1,1985)	1:136:A:TYR:HD1	1:135:A:TYR:H	5	0.94
(1,1985)	1:136:A:TYR:HD2	1:135:A:TYR:H	5	0.94
(1,1956)	1:34:A:GLU:HB2	1:36:A:GLN:H	4	0.94
(1,1956)	1:34:A:GLU:HB3	1:36:A:GLN:H	4	0.94
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	7	0.94
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	6	0.94
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	6	0.94
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	9	0.94
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	4	0.94
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	5	0.94
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	8	0.94
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE1	2	0.94
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE2	2	0.94
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE3	2	0.94
(1,450)	1:155:A:GLN:HG3	1:159:A:GLY:H	5	0.94
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	5	0.94
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	7	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	7	0.94
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	7	0.94
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	7	0.94
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	7	0.94
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	7	0.94
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD11	7	0.93
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD12	7	0.93
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD13	7	0.93
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	3	0.93
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	3	0.93
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	3	0.93
(1,3297)	1:143:A:GLN:HE22	1:142:A:LEU:H	9	0.93
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	10	0.93
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	10	0.93
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	10	0.93
(1,2786)	1:14:A:ILE:HG13	1:22:A:TRP:HE1	9	0.93
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	3	0.93
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	3	0.93
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	3	0.93
(1,1951)	1:184:A:LYS:HE3	1:184:A:LYS:HA	1	0.93
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	5	0.93
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	5	0.93
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	5	0.93
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	5	0.93
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	5	0.93
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	5	0.93
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	5	0.93
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	5	0.93
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	5	0.93
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD11	5	0.93
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD12	5	0.93
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD13	5	0.93
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	10	0.93
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	10	0.93
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	10	0.93
(1,420)	1:136:A:TYR:HB3	1:119:A:SER:H	1	0.93
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	7	0.93
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	7	0.93
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	7	0.93
(1,316)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	9	0.93
(1,316)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	9	0.93
(1,316)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	9	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	9	0.93
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	9	0.93
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	9	0.93
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	2	0.93
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	2	0.93
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	2	0.93
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	10	0.93
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	10	0.93
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	10	0.93
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	8	0.93
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	8	0.93
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	8	0.93
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	8	0.93
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	8	0.93
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	8	0.93
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	1	0.93
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	1	0.93
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	1	0.93
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	1	0.93
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	1	0.93
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	1	0.93
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	1	0.93
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	1	0.93
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	1	0.93
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	4	0.92
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	4	0.92
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	10	0.92
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	10	0.92
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	10	0.92
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	1	0.92
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD1	1	0.92
(1,2727)	1:1:A:MET:HE1	1:70:A:PHE:HD2	1	0.92
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD1	1	0.92
(1,2727)	1:1:A:MET:HE2	1:70:A:PHE:HD2	1	0.92
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD1	1	0.92
(1,2727)	1:1:A:MET:HE3	1:70:A:PHE:HD2	1	0.92
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	2	0.92
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	4	0.92
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	6	0.92
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	5	0.92
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	8	0.92
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD11	4	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD12	4	0.92
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD13	4	0.92
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD11	4	0.92
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD12	4	0.92
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD13	4	0.92
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD11	4	0.92
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD12	4	0.92
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD13	4	0.92
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	10	0.92
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	3	0.92
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	5	0.92
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	3	0.92
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	8	0.92
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	8	0.92
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	8	0.92
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG21	1	0.92
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG22	1	0.92
(1,613)	1:158:A:HIS:HD2	1:94:A:VAL:HG23	1	0.92
(1,333)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	10	0.92
(1,333)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	10	0.92
(1,333)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	10	0.92
(1,245)	1:69:A:MET:HE1	1:68:A:GLN:H	8	0.92
(1,245)	1:69:A:MET:HE2	1:68:A:GLN:H	8	0.92
(1,245)	1:69:A:MET:HE3	1:68:A:GLN:H	8	0.92
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	5	0.92
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	5	0.92
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	5	0.92
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	5	0.92
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	5	0.92
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	5	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG11	1	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG12	1	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG13	1	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG11	3	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG12	3	0.92
(1,40)	1:21:A:VAL:HB	1:58:A:VAL:HG13	3	0.92
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB2	3	0.92
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB3	3	0.92
(2,4)	1:139:A:ARG:HH21	2:201:A:Z90:OAB	1	0.91
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	5	0.91
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	5	0.91
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	5	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	1	0.91
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	1	0.91
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	1	0.91
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	10	0.91
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	2	0.91
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	4	0.91
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG11	6	0.91
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG12	6	0.91
(1,2715)	1:59:A:LEU:HB2	1:58:A:VAL:HG13	6	0.91
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG11	6	0.91
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG12	6	0.91
(1,2715)	1:59:A:LEU:HB3	1:58:A:VAL:HG13	6	0.91
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	3	0.91
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	3	0.91
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	3	0.91
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	4	0.91
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	10	0.91
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	10	0.91
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	10	0.91
(1,2017)	1:136:A:TYR:HB2	1:119:A:SER:H	2	0.91
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	4	0.91
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	4	0.91
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	4	0.91
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	4	0.91
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	4	0.91
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	4	0.91
(1,1864)	1:38:A:LEU:HB2	1:41:A:ILE:H	2	0.91
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	9	0.91
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	3	0.91
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	3	0.91
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	3	0.91
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	3	0.91
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	3	0.91
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	3	0.91
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	8	0.91
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	8	0.91
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	8	0.91
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	8	0.91
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	8	0.91
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	8	0.91
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	8	0.91
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	8	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	8	0.91
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	8	0.91
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	8	0.91
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	8	0.91
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	5	0.91
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	5	0.91
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	5	0.91
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	5	0.91
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	5	0.91
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	5	0.91
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	2	0.91
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	2	0.91
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	2	0.91
(1,3484)	1:37:A:PHE:H	1:35:A:GLY:H	6	0.9
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD21	2	0.9
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD22	2	0.9
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD23	2	0.9
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	10	0.9
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	8	0.9
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	8	0.9
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	8	0.9
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	1	0.9
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	3	0.9
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	3	0.9
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	3	0.9
(1,2267)	1:155:A:GLN:HG2	1:160:A:THR:H	9	0.9
(1,2266)	1:171:A:ASN:HD22	1:173:A:GLU:H	4	0.9
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	4	0.9
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	4	0.9
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	4	0.9
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE1	6	0.9
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE2	6	0.9
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE3	6	0.9
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG21	9	0.9
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG22	9	0.9
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG23	9	0.9
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG21	9	0.9
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG22	9	0.9
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG23	9	0.9
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG21	9	0.9
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG22	9	0.9
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG23	9	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	9	0.9
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	9	0.9
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	9	0.9
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	9	0.9
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	9	0.9
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	9	0.9
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	9	0.9
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	9	0.9
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	9	0.9
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	3	0.9
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	5	0.9
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	5	0.9
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	5	0.9
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	9	0.9
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	3	0.9
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	3	0.9
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	3	0.9
(1,212)	1:162:A:ILE:HG21	1:182:A:GLU:H	4	0.9
(1,212)	1:162:A:ILE:HG22	1:182:A:GLU:H	4	0.9
(1,212)	1:162:A:ILE:HG23	1:182:A:GLU:H	4	0.9
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	8	0.9
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	8	0.9
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	8	0.9
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	8	0.9
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	8	0.9
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	8	0.9
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB2	3	0.9
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB3	3	0.9
(1,3372)	1:122:A:CYS:HA	1:98:A:LEU:HD21	9	0.89
(1,3372)	1:122:A:CYS:HA	1:98:A:LEU:HD22	9	0.89
(1,3372)	1:122:A:CYS:HA	1:98:A:LEU:HD23	9	0.89
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	6	0.89
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	6	0.89
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	6	0.89
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	4	0.89
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	6	0.89
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	3	0.89
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	3	0.89
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	3	0.89
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD21	5	0.89
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD22	5	0.89
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD23	5	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2577)	1:128:A:GLY:HA3	1:130:A:GLY:H	5	0.89
(1,2301)	1:136:A:TYR:HA	1:119:A:SER:H	1	0.89
(1,2125)	1:136:A:TYR:HA	1:119:A:SER:H	1	0.89
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD21	6	0.89
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD22	6	0.89
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD23	6	0.89
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD21	6	0.89
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD22	6	0.89
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD23	6	0.89
(1,1439)	1:99:A:GLN:HE22	1:95:A:ARG:HG2	1	0.89
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	2	0.89
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	4	0.89
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	1	0.89
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	3	0.89
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	4	0.89
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	9	0.89
(1,462)	1:165:A:LYS:HD3	1:180:A:LEU:H	3	0.89
(1,454)	1:176:A:HIS:H	1:170:A:ARG:HA	2	0.89
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG21	7	0.89
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG22	7	0.89
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG23	7	0.89
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	5	0.89
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	5	0.89
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	5	0.89
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	4	0.89
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	4	0.89
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	4	0.89
(1,288)	1:39:A:VAL:HG21	2:201:A:Z90:HAJ	1	0.89
(1,288)	1:39:A:VAL:HG22	2:201:A:Z90:HAJ	1	0.89
(1,288)	1:39:A:VAL:HG23	2:201:A:Z90:HAJ	1	0.89
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG21	4	0.89
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG22	4	0.89
(1,227)	1:63:A:ALA:H	1:66:A:ILE:HG23	4	0.89
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	7	0.89
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	7	0.89
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD21	10	0.88
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD22	10	0.88
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD23	10	0.88
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD21	10	0.88
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD22	10	0.88
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD23	10	0.88
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	4	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	4	0.88
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	4	0.88
(1,2415)	1:75:A:PHE:HE1	1:156:A:GLN:H	1	0.88
(1,2415)	1:75:A:PHE:HE2	1:156:A:GLN:H	1	0.88
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	10	0.88
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	7	0.88
(1,2192)	1:65:A:GLU:HG2	1:63:A:ALA:H	9	0.88
(1,2192)	1:65:A:GLU:HG3	1:63:A:ALA:H	9	0.88
(1,2169)	1:186:A:SER:H	1:184:A:LYS:HA	2	0.88
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	8	0.88
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	8	0.88
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	8	0.88
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	3	0.88
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	6	0.88
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	6	0.88
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	6	0.88
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	9	0.88
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	2	0.88
(1,1396)	1:158:A:HIS:HD2	1:154:A:ALA:HA	8	0.88
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	4	0.88
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	1	0.88
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	1	0.88
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	1	0.88
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	1	0.88
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	1	0.88
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	1	0.88
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	7	0.88
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	7	0.88
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	7	0.88
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	3	0.88
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	3	0.88
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	3	0.88
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	10	0.88
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	10	0.88
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	10	0.88
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	10	0.88
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	10	0.88
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	10	0.88
(1,3456)	1:158:A:HIS:HD2	1:94:A:VAL:HA	2	0.87
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	9	0.87
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	9	0.87
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	8	0.87
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG11	6	0.87
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG12	6	0.87
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG13	6	0.87
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	2	0.87
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	2	0.87
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	2	0.87
(1,2460)	1:138:A:GLU:H	1:118:A:PRO:HA	8	0.87
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	1	0.87
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD21	1	0.87
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD22	1	0.87
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD23	1	0.87
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	5	0.87
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	10	0.87
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD11	8	0.87
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD12	8	0.87
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD13	8	0.87
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	10	0.87
(1,593)	1:170:A:ARG:HG3	1:171:A:ASN:H	7	0.87
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	5	0.87
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	5	0.87
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	5	0.87
(1,462)	1:165:A:LYS:HD3	1:180:A:LEU:H	6	0.87
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	6	0.87
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	8	0.87
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD21	1	0.87
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD22	1	0.87
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD23	1	0.87
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	7	0.86
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	7	0.86
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	7	0.86
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG21	9	0.86
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG22	9	0.86
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG23	9	0.86
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	2	0.86
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	2	0.86
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	2	0.86
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	2	0.86
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	5	0.86
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	2	0.86
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	2	0.86
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	2	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	4	0.86
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	4	0.86
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	4	0.86
(1,579)	1:173:A:GLU:HB2	1:171:A:ASN:H	1	0.86
(1,245)	1:69:A:MET:HE1	1:68:A:GLN:H	3	0.86
(1,245)	1:69:A:MET:HE2	1:68:A:GLN:H	3	0.86
(1,245)	1:69:A:MET:HE3	1:68:A:GLN:H	3	0.86
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB2	6	0.86
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB3	6	0.86
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	3	0.85
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	7	0.85
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	5	0.85
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG21	7	0.85
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG22	7	0.85
(1,2559)	1:59:A:LEU:HD21	1:66:A:ILE:HG23	7	0.85
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG21	7	0.85
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG22	7	0.85
(1,2559)	1:59:A:LEU:HD22	1:66:A:ILE:HG23	7	0.85
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG21	7	0.85
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG22	7	0.85
(1,2559)	1:59:A:LEU:HD23	1:66:A:ILE:HG23	7	0.85
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	4	0.85
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	4	0.85
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	4	0.85
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD21	2	0.85
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD22	2	0.85
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD23	2	0.85
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	5	0.85
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	5	0.85
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	5	0.85
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	2	0.85
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	2	0.85
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	2	0.85
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	4	0.85
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	4	0.85
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	6	0.85
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	6	0.85
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	6	0.85
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	9	0.85
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	10	0.85
(1,335)	1:101:A:LEU:HD11	2:201:A:Z90:HAH	10	0.85
(1,335)	1:101:A:LEU:HD12	2:201:A:Z90:HAH	10	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:101:A:LEU:HD13	2:201:A:Z90:HAH	10	0.85
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	4	0.85
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	4	0.85
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	4	0.85
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	4	0.85
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	4	0.85
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	4	0.85
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	1	0.85
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	1	0.85
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	1	0.85
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	1	0.84
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	1	0.84
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	1	0.84
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	5	0.84
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	5	0.84
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	10	0.84
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	10	0.84
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	10	0.84
(1,2896)	1:136:A:TYR:H	1:119:A:SER:H	9	0.84
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	4	0.84
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	4	0.84
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	4	0.84
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD11	7	0.84
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD12	7	0.84
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD13	7	0.84
(1,2781)	1:9:A:LEU:HD21	1:13:A:VAL:H	3	0.84
(1,2781)	1:9:A:LEU:HD22	1:13:A:VAL:H	3	0.84
(1,2781)	1:9:A:LEU:HD23	1:13:A:VAL:H	3	0.84
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	10	0.84
(1,1960)	1:184:A:LYS:HE2	1:184:A:LYS:HA	5	0.84
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB1	5	0.84
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB2	5	0.84
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB3	5	0.84
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	7	0.84
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	3	0.84
(1,1459)	1:79:A:GLN:HB2	1:82:A:GLY:H	7	0.84
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD11	7	0.84
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD12	7	0.84
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD13	7	0.84
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	6	0.84
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	6	0.84
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	6	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	1	0.84
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	1	0.84
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	1	0.84
(1,471)	1:26:A:LYS:HB3	1:25:A:ILE:H	7	0.84
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	6	0.84
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	6	0.84
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	6	0.84
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	4	0.84
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD21	7	0.83
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD22	7	0.83
(1,3281)	1:26:A:LYS:HA	1:31:A:LEU:HD23	7	0.83
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	3	0.83
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG21	2	0.83
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG22	2	0.83
(1,2809)	1:168:A:GLN:H	1:177:A:THR:HG23	2	0.83
(1,2743)	1:62:A:ASN:HD22	1:65:A:GLU:HB2	1	0.83
(1,2743)	1:62:A:ASN:HD22	1:65:A:GLU:HB3	1	0.83
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	9	0.83
(1,2198)	1:37:A:PHE:HD1	1:6:A:ASN:H	7	0.83
(1,2198)	1:37:A:PHE:HD2	1:6:A:ASN:H	7	0.83
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	3	0.83
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE1	7	0.83
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE2	7	0.83
(1,1566)	2:201:A:Z90:HAF	1:115:A:MET:HE3	7	0.83
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	6	0.83
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	8	0.83
(1,1311)	1:162:A:ILE:HG13	1:155:A:GLN:H	8	0.83
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	3	0.83
(1,994)	1:165:A:LYS:HE3	1:180:A:LEU:H	8	0.83
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	8	0.83
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	8	0.83
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	8	0.83
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	9	0.83
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	3	0.83
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	3	0.83
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	3	0.83
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	3	0.83
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	3	0.83
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	3	0.83
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	6	0.83
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	6	0.83
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:174:A:CYS:H	1:170:A:ARG:HA	4	0.83
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	6	0.82
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	6	0.82
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	6	0.82
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	3	0.82
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	3	0.82
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	6	0.82
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	6	0.82
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD21	7	0.82
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD22	7	0.82
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD23	7	0.82
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	1	0.82
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	3	0.82
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	3	0.82
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	3	0.82
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	4	0.82
(1,1704)	1:184:A:LYS:HD2	1:161:A:GLU:H	4	0.82
(1,1704)	1:184:A:LYS:HD3	1:161:A:GLU:H	4	0.82
(1,1479)	1:82:A:GLY:H	1:78:A:CYS:HA	7	0.82
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	3	0.82
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	8	0.82
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	8	0.82
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	8	0.82
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	8	0.82
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD21	9	0.82
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD22	9	0.82
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD23	9	0.82
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD11	8	0.82
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD12	8	0.82
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD13	8	0.82
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD11	8	0.82
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD12	8	0.82
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD13	8	0.82
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD11	8	0.82
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD12	8	0.82
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD13	8	0.82
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	7	0.82
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	7	0.82
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	7	0.82
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	6	0.82
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	6	0.82
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	2	0.82
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	2	0.82
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	2	0.82
(1,3563)	1:131:A:LEU:HB3	1:181:A:ILE:H	3	0.81
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	3	0.81
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	3	0.81
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	3	0.81
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	6	0.81
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	6	0.81
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	6	0.81
(1,2755)	1:65:A:GLU:H	1:66:A:ILE:HG12	5	0.81
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	3	0.81
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	8	0.81
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	7	0.81
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	7	0.81
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	7	0.81
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	4	0.81
(1,2266)	1:171:A:ASN:HD22	1:173:A:GLU:H	9	0.81
(1,2252)	1:155:A:GLN:HG3	1:160:A:THR:H	8	0.81
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	4	0.81
(1,1951)	1:184:A:LYS:HE3	1:184:A:LYS:HA	7	0.81
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	8	0.81
(1,1825)	1:96:A:GLU:HG3	1:93:A:ASN:H	2	0.81
(1,1817)	1:66:A:ILE:HB	1:56:A:SER:H	1	0.81
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	1	0.81
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	10	0.81
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	8	0.81
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	8	0.81
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	8	0.81
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD21	10	0.81
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD22	10	0.81
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD23	10	0.81
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	7	0.81
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	10	0.81
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	7	0.81
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	7	0.81
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	7	0.81
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE1	4	0.81
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE2	4	0.81
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE1	4	0.81
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE2	4	0.81
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE1	4	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE2	4	0.81
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD21	1	0.81
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD22	1	0.81
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD23	1	0.81
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD21	1	0.81
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD22	1	0.81
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD23	1	0.81
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD21	1	0.81
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD22	1	0.81
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD23	1	0.81
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	9	0.81
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	9	0.81
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	9	0.81
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	8	0.81
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	3	0.81
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	3	0.81
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	3	0.81
(1,265)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	9	0.81
(1,265)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	9	0.81
(1,265)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	9	0.81
(1,245)	1:66:A:ILE:HB	1:68:A:GLN:H	9	0.81
(1,82)	1:19:A:PRO:HG2	1:21:A:VAL:H	9	0.81
(1,82)	1:19:A:PRO:HG3	1:21:A:VAL:H	9	0.81
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD11	10	0.81
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD12	10	0.81
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD13	10	0.81
(1,3526)	1:12:A:LEU:HA	1:16:A:ASN:HD22	5	0.8
(1,3457)	1:188:A:GLU:H	1:186:A:SER:HA	8	0.8
(1,3384)	1:120:A:PHE:HD1	1:135:A:TYR:H	5	0.8
(1,3384)	1:120:A:PHE:HD2	1:135:A:TYR:H	5	0.8
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	2	0.8
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	2	0.8
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	2	0.8
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	8	0.8
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD21	3	0.8
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD22	3	0.8
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD23	3	0.8
(1,2798)	1:10:A:GLU:HA	1:22:A:TRP:HE1	9	0.8
(1,2771)	1:137:A:SER:HA	1:119:A:SER:H	7	0.8
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	2	0.8
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	2	0.8
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	2	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	7	0.8
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	7	0.8
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	8	0.8
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	10	0.8
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	9	0.8
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	8	0.8
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	8	0.8
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	8	0.8
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	10	0.8
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	10	0.8
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	10	0.8
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	5	0.8
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	5	0.8
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	5	0.8
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG21	1	0.8
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG22	1	0.8
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG23	1	0.8
(1,959)	1:59:A:LEU:HD21	1:58:A:VAL:HG21	2	0.8
(1,959)	1:59:A:LEU:HD21	1:58:A:VAL:HG22	2	0.8
(1,959)	1:59:A:LEU:HD21	1:58:A:VAL:HG23	2	0.8
(1,959)	1:59:A:LEU:HD22	1:58:A:VAL:HG21	2	0.8
(1,959)	1:59:A:LEU:HD22	1:58:A:VAL:HG22	2	0.8
(1,959)	1:59:A:LEU:HD22	1:58:A:VAL:HG23	2	0.8
(1,959)	1:59:A:LEU:HD23	1:58:A:VAL:HG21	2	0.8
(1,959)	1:59:A:LEU:HD23	1:58:A:VAL:HG22	2	0.8
(1,959)	1:59:A:LEU:HD23	1:58:A:VAL:HG23	2	0.8
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	3	0.8
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	3	0.8
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	3	0.8
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	3	0.8
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	5	0.8
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	5	0.8
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	5	0.8
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	1	0.8
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	1	0.8
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	1	0.8
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	8	0.8
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	8	0.8
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	4	0.8
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	4	0.8
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	4	0.8
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	4	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	4	0.8
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	4	0.8
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	6	0.8
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	6	0.8
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	5	0.8
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	5	0.8
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	5	0.8
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	5	0.8
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	5	0.8
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	5	0.8
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	5	0.8
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	5	0.8
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	5	0.8
(1,3484)	1:37:A:PHE:H	1:35:A:GLY:H	8	0.79
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD21	4	0.79
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD22	4	0.79
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD23	4	0.79
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD21	1	0.79
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD22	1	0.79
(1,2747)	1:1:A:MET:HE1	1:9:A:LEU:HD23	1	0.79
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD21	1	0.79
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD22	1	0.79
(1,2747)	1:1:A:MET:HE2	1:9:A:LEU:HD23	1	0.79
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD21	1	0.79
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD22	1	0.79
(1,2747)	1:1:A:MET:HE3	1:9:A:LEU:HD23	1	0.79
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	8	0.79
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	8	0.79
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	8	0.79
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	6	0.79
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	9	0.79
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	9	0.79
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	9	0.79
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	9	0.79
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	9	0.79
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	9	0.79
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	1	0.79
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	2	0.79
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	6	0.79
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	6	0.79
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	6	0.79
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	1	0.79
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	1	0.79
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD11	4	0.79
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD12	4	0.79
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD13	4	0.79
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	8	0.79
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	8	0.79
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	8	0.79
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD11	7	0.79
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD12	7	0.79
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD13	7	0.79
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	3	0.79
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	3	0.79
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	3	0.79
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	2	0.79
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	2	0.79
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	2	0.79
(1,3461)	1:132:A:ILE:HG12	1:125:A:ALA:H	5	0.78
(1,3384)	1:120:A:PHE:HD1	1:135:A:TYR:H	4	0.78
(1,3384)	1:120:A:PHE:HD2	1:135:A:TYR:H	4	0.78
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	1	0.78
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	6	0.78
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	9	0.78
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG21	3	0.78
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG22	3	0.78
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG23	3	0.78
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	4	0.78
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	5	0.78
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	5	0.78
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	5	0.78
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	10	0.78
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	7	0.78
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	7	0.78
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	7	0.78
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	1	0.78
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	7	0.78
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	4	0.78
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	6	0.78
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	4	0.78
(1,735)	1:157:A:ILE:HB	1:159:A:GLY:H	6	0.78
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	6	0.78
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	6	0.78
(1,645)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	10	0.78
(1,593)	1:170:A:ARG:HG3	1:171:A:ASN:H	2	0.78
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	6	0.78
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	10	0.78
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	10	0.78
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	10	0.78
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	10	0.78
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	10	0.78
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	10	0.78
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD1	7	0.78
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD2	7	0.78
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD1	7	0.78
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD2	7	0.78
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD1	7	0.78
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD2	7	0.78
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	9	0.77
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	2	0.77
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	3	0.77
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	3	0.77
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	3	0.77
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	10	0.77
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	10	0.77
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	10	0.77
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	7	0.77
(1,2188)	1:183:A:GLU:HB2	1:185:A:GLU:H	10	0.77
(1,2128)	1:59:A:LEU:HD21	1:21:A:VAL:HG21	2	0.77
(1,2128)	1:59:A:LEU:HD21	1:21:A:VAL:HG22	2	0.77
(1,2128)	1:59:A:LEU:HD21	1:21:A:VAL:HG23	2	0.77
(1,2128)	1:59:A:LEU:HD22	1:21:A:VAL:HG21	2	0.77
(1,2128)	1:59:A:LEU:HD22	1:21:A:VAL:HG22	2	0.77
(1,2128)	1:59:A:LEU:HD22	1:21:A:VAL:HG23	2	0.77
(1,2128)	1:59:A:LEU:HD23	1:21:A:VAL:HG21	2	0.77
(1,2128)	1:59:A:LEU:HD23	1:21:A:VAL:HG22	2	0.77
(1,2128)	1:59:A:LEU:HD23	1:21:A:VAL:HG23	2	0.77
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG21	5	0.77
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG22	5	0.77
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG23	5	0.77
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	2	0.77
(1,1874)	1:170:A:ARG:HE	1:177:A:THR:H	8	0.77
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB1	8	0.77
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB2	8	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB3	8	0.77
(1,1324)	1:84:A:ASP:HB3	1:83:A:TYR:H	3	0.77
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	10	0.77
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	10	0.77
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	10	0.77
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	8	0.77
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	8	0.77
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	8	0.77
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	3	0.77
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG21	3	0.77
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG22	3	0.77
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG23	3	0.77
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	3	0.77
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	3	0.77
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	3	0.77
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	1	0.77
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	1	0.77
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	1	0.77
(1,593)	1:170:A:ARG:HG3	1:171:A:ASN:H	6	0.77
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	2	0.77
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	10	0.77
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	10	0.77
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	10	0.77
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	10	0.77
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	10	0.77
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	10	0.77
(1,137)	1:56:A:SER:HB2	1:62:A:ASN:H	3	0.77
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE1	2	0.77
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE2	2	0.77
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE3	2	0.77
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD1	4	0.77
(1,24)	1:1:A:MET:HE1	1:49:A:TYR:HD2	4	0.77
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD1	4	0.77
(1,24)	1:1:A:MET:HE2	1:49:A:TYR:HD2	4	0.77
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD1	4	0.77
(1,24)	1:1:A:MET:HE3	1:49:A:TYR:HD2	4	0.77
(1,3460)	1:101:A:LEU:HD21	1:98:A:LEU:HD11	4	0.76
(1,3460)	1:101:A:LEU:HD21	1:98:A:LEU:HD12	4	0.76
(1,3460)	1:101:A:LEU:HD21	1:98:A:LEU:HD13	4	0.76
(1,3460)	1:101:A:LEU:HD22	1:98:A:LEU:HD11	4	0.76
(1,3460)	1:101:A:LEU:HD22	1:98:A:LEU:HD12	4	0.76
(1,3460)	1:101:A:LEU:HD22	1:98:A:LEU:HD13	4	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3460)	1:101:A:LEU:HD23	1:98:A:LEU:HD11	4	0.76
(1,3460)	1:101:A:LEU:HD23	1:98:A:LEU:HD12	4	0.76
(1,3460)	1:101:A:LEU:HD23	1:98:A:LEU:HD13	4	0.76
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	5	0.76
(1,2863)	1:126:A:GLU:H	1:130:A:GLY:H	4	0.76
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	6	0.76
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	6	0.76
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	6	0.76
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD1	8	0.76
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD2	8	0.76
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	7	0.76
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	3	0.76
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	3	0.76
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	3	0.76
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	6	0.76
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	6	0.76
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	6	0.76
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	5	0.76
(1,1953)	1:175:A:ASP:H	1:170:A:ARG:HG2	3	0.76
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	3	0.76
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	2	0.76
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	9	0.76
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	9	0.76
(1,1172)	1:135:A:TYR:HD1	1:177:A:THR:H	6	0.76
(1,1172)	1:135:A:TYR:HD2	1:177:A:THR:H	6	0.76
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	1	0.76
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	4	0.76
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	7	0.76
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	7	0.76
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	7	0.76
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	4	0.76
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	4	0.76
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	4	0.76
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	2	0.76
(1,463)	1:59:A:LEU:HD11	1:55:A:ALA:HB1	2	0.76
(1,463)	1:59:A:LEU:HD11	1:55:A:ALA:HB2	2	0.76
(1,463)	1:59:A:LEU:HD11	1:55:A:ALA:HB3	2	0.76
(1,463)	1:59:A:LEU:HD12	1:55:A:ALA:HB1	2	0.76
(1,463)	1:59:A:LEU:HD12	1:55:A:ALA:HB2	2	0.76
(1,463)	1:59:A:LEU:HD12	1:55:A:ALA:HB3	2	0.76
(1,463)	1:59:A:LEU:HD13	1:55:A:ALA:HB1	2	0.76
(1,463)	1:59:A:LEU:HD13	1:55:A:ALA:HB2	2	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:59:A:LEU:HD13	1:55:A:ALA:HB3	2	0.76
(1,462)	1:165:A:LYS:HD3	1:180:A:LEU:H	2	0.76
(1,454)	1:176:A:HIS:H	1:170:A:ARG:HA	10	0.76
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	1	0.76
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	1	0.76
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	1	0.76
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	7	0.76
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	7	0.76
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	7	0.76
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	7	0.76
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	7	0.76
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	7	0.76
(1,82)	1:19:A:PRO:HG2	1:21:A:VAL:H	6	0.76
(1,82)	1:19:A:PRO:HG3	1:21:A:VAL:H	6	0.76
(1,3354)	1:27:A:LYS:HD3	1:28:A:GLU:H	2	0.75
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	3	0.75
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	3	0.75
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	3	0.75
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	3	0.75
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	10	0.75
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	10	0.75
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	10	0.75
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	6	0.75
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	6	0.75
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	6	0.75
(1,2212)	1:184:A:LYS:HD2	1:184:A:LYS:H	3	0.75
(1,2212)	1:184:A:LYS:HD3	1:184:A:LYS:H	3	0.75
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	1	0.75
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	3	0.75
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	9	0.75
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	9	0.75
(1,1404)	1:50:A:ASP:HB3	1:49:A:TYR:H	8	0.75
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	4	0.75
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	4	0.75
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	4	0.75
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	9	0.75
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	9	0.75
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	9	0.75
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD11	8	0.75
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD12	8	0.75
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD13	8	0.75
(1,1297)	1:145:A:ILE:HG12	1:71:A:GLY:H	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:100:A:ASN:HB3	1:99:A:GLN:H	6	0.75
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	5	0.75
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	5	0.75
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	5	0.75
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	3	0.75
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	7	0.75
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	7	0.75
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	7	0.75
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	2	0.75
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	2	0.75
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	2	0.75
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	9	0.75
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	9	0.75
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	9	0.75
(1,3284)	1:100:A:ASN:HB3	1:103:A:ALA:H	4	0.74
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD11	1	0.74
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD12	1	0.74
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD13	1	0.74
(1,3107)	1:24:A:ASP:HB3	1:22:A:TRP:H	1	0.74
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	9	0.74
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD11	10	0.74
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD12	10	0.74
(1,2800)	2:201:A:Z90:HAH	1:101:A:LEU:HD13	10	0.74
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	2	0.74
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	2	0.74
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	2	0.74
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	3	0.74
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG12	6	0.74
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG13	6	0.74
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	4	0.74
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	8	0.74
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	2	0.74
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	4	0.74
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	4	0.74
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD11	2	0.74
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD12	2	0.74
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD13	2	0.74
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	6	0.74
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	6	0.74
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	6	0.74
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	6	0.74
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	6	0.74
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	6	0.74
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	6	0.74
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	6	0.74
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	2	0.74
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	2	0.74
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	2	0.74
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	9	0.74
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	9	0.74
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	9	0.74
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	2	0.74
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	2	0.74
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	2	0.74
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD11	7	0.74
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD12	7	0.74
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD13	7	0.74
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD11	7	0.74
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD12	7	0.74
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD13	7	0.74
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD11	7	0.74
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD12	7	0.74
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD13	7	0.74
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG21	10	0.74
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG22	10	0.74
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG23	10	0.74
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE1	10	0.74
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE2	10	0.74
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE3	10	0.74
(1,335)	1:101:A:LEU:HD11	2:201:A:Z90:HAH	6	0.74
(1,335)	1:101:A:LEU:HD12	2:201:A:Z90:HAH	6	0.74
(1,335)	1:101:A:LEU:HD13	2:201:A:Z90:HAH	6	0.74
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	5	0.74
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	5	0.74
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	5	0.74
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	9	0.74
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	9	0.74
(1,82)	1:19:A:PRO:HG2	1:21:A:VAL:H	10	0.74
(1,82)	1:19:A:PRO:HG3	1:21:A:VAL:H	10	0.74
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD21	2	0.74
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD22	2	0.74
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD23	2	0.74
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD21	2	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD22	2	0.74
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD23	2	0.74
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD11	1	0.74
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD12	1	0.74
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD13	1	0.74
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD11	1	0.74
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD12	1	0.74
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD13	1	0.74
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD11	1	0.74
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD12	1	0.74
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD13	1	0.74
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	4	0.73
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	4	0.73
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	4	0.73
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	5	0.73
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	8	0.73
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	8	0.73
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	8	0.73
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	5	0.73
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	5	0.73
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	5	0.73
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	7	0.73
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	2	0.73
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	2	0.73
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	2	0.73
(1,2479)	1:92:A:SER:HB3	1:93:A:ASN:HD22	4	0.73
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD11	8	0.73
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD12	8	0.73
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD13	8	0.73
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	6	0.73
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	1	0.73
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	1	0.73
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	1	0.73
(1,2196)	1:164:A:MET:HA	1:165:A:LYS:HD2	6	0.73
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	2	0.73
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	2	0.73
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	2	0.73
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	2	0.73
(1,1928)	2:201:A:Z90:HAM	1:101:A:LEU:HD11	4	0.73
(1,1928)	2:201:A:Z90:HAM	1:101:A:LEU:HD12	4	0.73
(1,1928)	2:201:A:Z90:HAM	1:101:A:LEU:HD13	4	0.73
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	10	0.73
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	9	0.73
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	4	0.73
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD21	6	0.73
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD22	6	0.73
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD23	6	0.73
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	6	0.73
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	1	0.73
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	1	0.73
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	1	0.73
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD1	4	0.73
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD2	4	0.73
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	9	0.73
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	9	0.73
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	9	0.73
(1,864)	1:166:A:VAL:HB	1:178:A:GLN:H	6	0.73
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	8	0.73
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	8	0.73
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	8	0.73
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	2	0.73
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	2	0.73
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	2	0.73
(1,593)	1:170:A:ARG:HG3	1:171:A:ASN:H	10	0.73
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	3	0.73
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	3	0.73
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	3	0.73
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	3	0.73
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	3	0.73
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	3	0.73
(2,1)	1:135:A:TYR:HH	2:201:A:Z90:OAC	9	0.72
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	8	0.72
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	8	0.72
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	8	0.72
(1,3512)	1:140:A:GLU:HB2	1:169:A:GLN:HE22	9	0.72
(1,3254)	1:143:A:GLN:HE22	1:141:A:GLY:H	1	0.72
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	1	0.72
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	1	0.72
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	1	0.72
(1,3232)	1:32:A:ASP:HB3	1:27:A:LYS:H	1	0.72
(1,3218)	1:122:A:CYS:HB2	1:133:A:LEU:HD21	1	0.72
(1,3218)	1:122:A:CYS:HB2	1:133:A:LEU:HD22	1	0.72
(1,3218)	1:122:A:CYS:HB2	1:133:A:LEU:HD23	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3133)	1:60:A:ASN:HD22	1:60:A:ASN:H	4	0.72
(1,2957)	1:160:A:THR:H	1:94:A:VAL:HG21	1	0.72
(1,2957)	1:160:A:THR:H	1:94:A:VAL:HG22	1	0.72
(1,2957)	1:160:A:THR:H	1:94:A:VAL:HG23	1	0.72
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	7	0.72
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	7	0.72
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	7	0.72
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	8	0.72
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG11	7	0.72
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG12	7	0.72
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG13	7	0.72
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG11	7	0.72
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG12	7	0.72
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG13	7	0.72
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG11	7	0.72
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG12	7	0.72
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG13	7	0.72
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	5	0.72
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	5	0.72
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	5	0.72
(1,2139)	1:79:A:GLN:HA	1:84:A:ASP:H	7	0.72
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	6	0.72
(1,2092)	1:132:A:ILE:HD11	1:131:A:LEU:H	2	0.72
(1,2092)	1:132:A:ILE:HD12	1:131:A:LEU:H	2	0.72
(1,2092)	1:132:A:ILE:HD13	1:131:A:LEU:H	2	0.72
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	3	0.72
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	6	0.72
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	10	0.72
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	10	0.72
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	10	0.72
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD21	10	0.72
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD22	10	0.72
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD23	10	0.72
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD21	10	0.72
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD22	10	0.72
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD23	10	0.72
(1,1396)	1:158:A:HIS:HD2	1:154:A:ALA:HA	1	0.72
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	8	0.72
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	8	0.72
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	8	0.72
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	1	0.72
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	7	0.72
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	7	0.72
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	7	0.72
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	7	0.72
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	7	0.72
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	7	0.72
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	7	0.72
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	7	0.72
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD11	6	0.72
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD12	6	0.72
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD13	6	0.72
(1,1116)	1:160:A:THR:HB	1:155:A:GLN:HA	5	0.72
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	9	0.72
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	9	0.72
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	9	0.72
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD21	5	0.72
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD22	5	0.72
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD23	5	0.72
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD21	5	0.72
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD22	5	0.72
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD23	5	0.72
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD21	5	0.72
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD22	5	0.72
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD23	5	0.72
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	1	0.72
(1,864)	1:166:A:VAL:HB	1:178:A:GLN:H	8	0.72
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	2	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	5	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	5	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	5	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	9	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	9	0.72
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	9	0.72
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	4	0.72
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	4	0.72
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	4	0.72
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD11	1	0.72
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD12	1	0.72
(1,655)	1:59:A:LEU:HD11	1:61:A:LEU:HD13	1	0.72
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD11	1	0.72
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD12	1	0.72
(1,655)	1:59:A:LEU:HD12	1:61:A:LEU:HD13	1	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD11	1	0.72
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD12	1	0.72
(1,655)	1:59:A:LEU:HD13	1:61:A:LEU:HD13	1	0.72
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	6	0.72
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	9	0.72
(1,401)	1:132:A:ILE:HA	1:125:A:ALA:H	5	0.72
(1,189)	1:2:A:TYR:HD1	1:6:A:ASN:H	8	0.72
(1,189)	1:2:A:TYR:HD2	1:6:A:ASN:H	8	0.72
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	1	0.72
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	1	0.72
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD11	1	0.72
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD12	1	0.72
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD13	1	0.72
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD11	1	0.72
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD12	1	0.72
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD13	1	0.72
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD11	1	0.72
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD12	1	0.72
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD13	1	0.72
(1,3509)	1:128:A:GLY:H	1:127:A:LYS:H	1	0.71
(1,3133)	1:60:A:ASN:HD22	1:60:A:ASN:H	7	0.71
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	10	0.71
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	7	0.71
(1,2969)	1:37:A:PHE:HD1	1:10:A:GLU:HG3	4	0.71
(1,2969)	1:37:A:PHE:HD2	1:10:A:GLU:HG3	4	0.71
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	9	0.71
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	9	0.71
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	9	0.71
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	5	0.71
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	5	0.71
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	5	0.71
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	9	0.71
(1,2594)	1:171:A:ASN:HD22	1:174:A:CYS:H	4	0.71
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	5	0.71
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	5	0.71
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	5	0.71
(1,2017)	1:136:A:TYR:HB2	1:119:A:SER:H	9	0.71
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	9	0.71
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	6	0.71
(1,1825)	1:96:A:GLU:HG3	1:93:A:ASN:H	6	0.71
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	5	0.71
(1,1459)	1:79:A:GLN:HB2	1:82:A:GLY:H	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	2	0.71
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	9	0.71
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	9	0.71
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	9	0.71
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	9	0.71
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	9	0.71
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	9	0.71
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	9	0.71
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	9	0.71
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	9	0.71
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	5	0.71
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	5	0.71
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	5	0.71
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	7	0.71
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	7	0.71
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	7	0.71
(1,980)	1:62:A:ASN:HD22	1:61:A:LEU:HA	10	0.71
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	2	0.71
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	2	0.71
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	2	0.71
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	10	0.71
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	10	0.71
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	10	0.71
(1,524)	1:124:A:ASP:HB2	1:131:A:LEU:H	7	0.71
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	3	0.71
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	3	0.71
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB1	3	0.71
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB2	3	0.71
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB3	3	0.71
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB1	3	0.71
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB2	3	0.71
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB3	3	0.71
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB1	3	0.71
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB2	3	0.71
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB3	3	0.71
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	3	0.7
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	3	0.7
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	3	0.7
(1,3456)	1:158:A:HIS:HD2	1:94:A:VAL:HA	6	0.7
(1,3354)	1:27:A:LYS:HD3	1:28:A:GLU:H	4	0.7
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	1	0.7
(1,3133)	1:60:A:ASN:HD22	1:60:A:ASN:H	10	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2819)	1:160:A:THR:HB	1:159:A:GLY:H	5	0.7
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	4	0.7
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	4	0.7
(1,1939)	1:183:A:GLU:HG3	1:163:A:ASP:H	4	0.7
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	9	0.7
(1,1659)	1:7:A:HIS:HB2	1:11:A:LEU:H	3	0.7
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD11	3	0.7
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD12	3	0.7
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD13	3	0.7
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD11	3	0.7
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD12	3	0.7
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD13	3	0.7
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD11	3	0.7
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD12	3	0.7
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD13	3	0.7
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	3	0.7
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	3	0.7
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	3	0.7
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	6	0.7
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	6	0.7
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	6	0.7
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	4	0.7
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	4	0.7
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	4	0.7
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	4	0.7
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	4	0.7
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	4	0.7
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	4	0.7
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	4	0.7
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	4	0.7
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	4	0.7
(1,892)	1:172:A:GLU:H	1:171:A:ASN:HD22	1	0.7
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	8	0.7
(1,548)	1:143:A:GLN:HE22	1:144:A:ASP:H	3	0.7
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	9	0.7
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	9	0.7
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	9	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	2	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	2	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	2	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	2	0.7
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	2	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	2	0.7
(1,30)	1:41:A:ILE:HA	1:42:A:ILE:HG21	7	0.7
(1,30)	1:41:A:ILE:HA	1:42:A:ILE:HG22	7	0.7
(1,30)	1:41:A:ILE:HA	1:42:A:ILE:HG23	7	0.7
(1,3503)	1:135:A:TYR:HE1	1:119:A:SER:H	10	0.69
(1,3503)	1:135:A:TYR:HE2	1:119:A:SER:H	10	0.69
(1,3435)	1:146:A:VAL:HB	1:144:A:ASP:H	9	0.69
(1,3297)	1:143:A:GLN:HE22	1:142:A:LEU:H	10	0.69
(1,2871)	1:181:A:ILE:H	1:130:A:GLY:H	4	0.69
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	3	0.69
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	3	0.69
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	3	0.69
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	10	0.69
(1,2552)	1:99:A:GLN:HE22	1:96:A:GLU:H	4	0.69
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	6	0.69
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG21	6	0.69
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG22	6	0.69
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG23	6	0.69
(1,2025)	1:47:A:LYS:HE2	1:47:A:LYS:H	5	0.69
(1,1992)	1:92:A:SER:HB2	1:93:A:ASN:HD22	6	0.69
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE1	7	0.69
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE2	7	0.69
(1,1782)	1:65:A:GLU:H	1:69:A:MET:HE3	7	0.69
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	5	0.69
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD11	7	0.69
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD12	7	0.69
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD13	7	0.69
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD21	7	0.69
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD22	7	0.69
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD23	7	0.69
(1,1665)	1:143:A:GLN:HG2	1:166:A:VAL:HG11	8	0.69
(1,1665)	1:143:A:GLN:HG2	1:166:A:VAL:HG12	8	0.69
(1,1665)	1:143:A:GLN:HG2	1:166:A:VAL:HG13	8	0.69
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	1	0.69
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	2	0.69
(1,1495)	1:125:A:ALA:HB1	1:131:A:LEU:H	6	0.69
(1,1495)	1:125:A:ALA:HB2	1:131:A:LEU:H	6	0.69
(1,1495)	1:125:A:ALA:HB3	1:131:A:LEU:H	6	0.69
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	9	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	1	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	1	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	3	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	3	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	3	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	5	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	5	0.69
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	5	0.69
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD11	1	0.69
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD12	1	0.69
(1,1310)	1:145:A:ILE:H	1:67:A:LEU:HD13	1	0.69
(1,1156)	1:100:A:ASN:HB3	1:99:A:GLN:H	8	0.69
(1,1053)	1:162:A:ILE:HA	1:164:A:MET:H	1	0.69
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	7	0.69
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	7	0.69
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD11	8	0.69
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD12	8	0.69
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD13	8	0.69
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD11	8	0.69
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD12	8	0.69
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD13	8	0.69
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD11	8	0.69
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD12	8	0.69
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD13	8	0.69
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	10	0.69
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	3	0.69
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	3	0.69
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	3	0.69
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	10	0.69
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	10	0.69
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	10	0.69
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	3	0.69
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG11	7	0.69
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG12	7	0.69
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG13	7	0.69
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG11	9	0.69
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG12	9	0.69
(1,343)	2:201:A:Z90:HAR	1:5:A:VAL:HG13	9	0.69
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	4	0.69
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	4	0.69
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	4	0.69
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	9	0.69
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	9	0.69
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	6	0.69
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	6	0.69
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	6	0.69
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	6	0.69
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	6	0.69
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	6	0.69
(1,82)	1:19:A:PRO:HG2	1:21:A:VAL:H	7	0.69
(1,82)	1:19:A:PRO:HG3	1:21:A:VAL:H	7	0.69
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB2	1	0.69
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB3	1	0.69
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG21	6	0.68
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG22	6	0.68
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG23	6	0.68
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG21	6	0.68
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG22	6	0.68
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG23	6	0.68
(1,2899)	1:183:A:GLU:HG2	1:130:A:GLY:H	3	0.68
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	3	0.68
(1,2853)	1:176:A:HIS:HB2	1:137:A:SER:H	10	0.68
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	6	0.68
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	10	0.68
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	6	0.68
(1,2552)	1:99:A:GLN:HE22	1:96:A:GLU:H	6	0.68
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	2	0.68
(1,1900)	1:62:A:ASN:HD22	1:61:A:LEU:HA	10	0.68
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	4	0.68
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	2	0.68
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	5	0.68
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	1	0.68
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	1	0.68
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	1	0.68
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	1	0.68
(1,1388)	1:134:A:HIS:HD2	1:121:A:ARG:H	7	0.68
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD11	10	0.68
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD12	10	0.68
(1,1322)	1:145:A:ILE:HA	1:145:A:ILE:HD13	10	0.68
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	8	0.68
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	8	0.68
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	8	0.68
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	7	0.68
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	9	0.68
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	9	0.68
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	5	0.68
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	5	0.68
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	5	0.68
(1,824)	1:184:A:LYS:HE3	1:185:A:GLU:H	8	0.68
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	8	0.68
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	8	0.68
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	8	0.68
(1,600)	1:166:A:VAL:HG21	1:169:A:GLN:H	3	0.68
(1,600)	1:166:A:VAL:HG22	1:169:A:GLN:H	3	0.68
(1,600)	1:166:A:VAL:HG23	1:169:A:GLN:H	3	0.68
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	7	0.68
(1,593)	1:170:A:ARG:HG3	1:171:A:ASN:H	9	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	2	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	2	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	2	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	2	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	2	0.68
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	2	0.68
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	9	0.68
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	9	0.68
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	9	0.68
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	9	0.68
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	9	0.68
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	9	0.68
(2,4)	1:139:A:ARG:HH21	2:201:A:Z90:OAB	10	0.67
(1,3266)	1:75:A:PHE:HE1	1:157:A:ILE:HD11	5	0.67
(1,3266)	1:75:A:PHE:HE1	1:157:A:ILE:HD12	5	0.67
(1,3266)	1:75:A:PHE:HE1	1:157:A:ILE:HD13	5	0.67
(1,3266)	1:75:A:PHE:HE2	1:157:A:ILE:HD11	5	0.67
(1,3266)	1:75:A:PHE:HE2	1:157:A:ILE:HD12	5	0.67
(1,3266)	1:75:A:PHE:HE2	1:157:A:ILE:HD13	5	0.67
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	1	0.67
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	7	0.67
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	7	0.67
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	7	0.67
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	2	0.67
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	5	0.67
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	5	0.67
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	5	0.67
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	1	0.67
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	1	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	1	0.67
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG21	5	0.67
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG22	5	0.67
(1,2699)	1:155:A:GLN:H	1:153:A:VAL:HG23	5	0.67
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	7	0.67
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	7	0.67
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	7	0.67
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	6	0.67
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	6	0.67
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	6	0.67
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD11	7	0.67
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD12	7	0.67
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD13	7	0.67
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	5	0.67
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	1	0.67
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	1	0.67
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	1	0.67
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	4	0.67
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	4	0.67
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	4	0.67
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	5	0.67
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG21	2	0.67
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG22	2	0.67
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG23	2	0.67
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG11	3	0.67
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG12	3	0.67
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG13	3	0.67
(1,1881)	1:63:A:ALA:HB1	1:67:A:LEU:HD11	9	0.67
(1,1881)	1:63:A:ALA:HB1	1:67:A:LEU:HD12	9	0.67
(1,1881)	1:63:A:ALA:HB1	1:67:A:LEU:HD13	9	0.67
(1,1881)	1:63:A:ALA:HB2	1:67:A:LEU:HD11	9	0.67
(1,1881)	1:63:A:ALA:HB2	1:67:A:LEU:HD12	9	0.67
(1,1881)	1:63:A:ALA:HB2	1:67:A:LEU:HD13	9	0.67
(1,1881)	1:63:A:ALA:HB3	1:67:A:LEU:HD11	9	0.67
(1,1881)	1:63:A:ALA:HB3	1:67:A:LEU:HD12	9	0.67
(1,1881)	1:63:A:ALA:HB3	1:67:A:LEU:HD13	9	0.67
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	4	0.67
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	10	0.67
(1,1725)	1:128:A:GLY:H	1:130:A:GLY:H	5	0.67
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG21	10	0.67
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG22	10	0.67
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG23	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG21	10	0.67
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG22	10	0.67
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG23	10	0.67
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG21	10	0.67
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG22	10	0.67
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG23	10	0.67
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	1	0.67
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	1	0.67
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	1	0.67
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	1	0.67
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	1	0.67
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	1	0.67
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	1	0.67
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	1	0.67
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	1	0.67
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	1	0.67
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	1	0.67
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	1	0.67
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	1	0.67
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	1	0.67
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	1	0.67
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	1	0.67
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	1	0.67
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	1	0.67
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	10	0.67
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD11	2	0.67
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD12	2	0.67
(1,844)	1:41:A:ILE:H	1:42:A:ILE:HD13	2	0.67
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	4	0.67
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	4	0.67
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	4	0.67
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	8	0.67
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	8	0.67
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	8	0.67
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG11	6	0.67
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG12	6	0.67
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG13	6	0.67
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	4	0.67
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	4	0.67
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	4	0.67
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD11	5	0.67
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD12	5	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD13	5	0.67
(1,318)	1:101:A:LEU:HD21	2:201:A:Z90:HAM	2	0.67
(1,318)	1:101:A:LEU:HD22	2:201:A:Z90:HAM	2	0.67
(1,318)	1:101:A:LEU:HD23	2:201:A:Z90:HAM	2	0.67
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	5	0.67
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	9	0.67
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	9	0.67
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	9	0.67
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	9	0.67
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	9	0.67
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	9	0.67
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	9	0.67
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	9	0.67
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	9	0.67
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	9	0.67
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	9	0.67
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	9	0.67
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG21	3	0.66
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG22	3	0.66
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG23	3	0.66
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG21	3	0.66
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG22	3	0.66
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG23	3	0.66
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG21	3	0.66
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG22	3	0.66
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG23	3	0.66
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD21	4	0.66
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD22	4	0.66
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD23	4	0.66
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD21	4	0.66
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD22	4	0.66
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD23	4	0.66
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD21	4	0.66
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD22	4	0.66
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD23	4	0.66
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	10	0.66
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	2	0.66
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	2	0.66
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	2	0.66
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	4	0.66
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	3	0.66
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	1	0.66
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB1	10	0.66
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB2	10	0.66
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB3	10	0.66
(1,2577)	1:128:A:GLY:HA3	1:130:A:GLY:H	2	0.66
(1,2340)	1:139:A:ARG:HG2	1:141:A:GLY:H	3	0.66
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	2	0.66
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	10	0.66
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	5	0.66
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	5	0.66
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	5	0.66
(1,2092)	1:132:A:ILE:HD11	1:131:A:LEU:H	5	0.66
(1,2092)	1:132:A:ILE:HD12	1:131:A:LEU:H	5	0.66
(1,2092)	1:132:A:ILE:HD13	1:131:A:LEU:H	5	0.66
(1,1953)	1:175:A:ASP:H	1:170:A:ARG:HG2	1	0.66
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG11	5	0.66
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG12	5	0.66
(1,1926)	1:152:A:THR:H	1:153:A:VAL:HG13	5	0.66
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	9	0.66
(1,1820)	1:56:A:SER:HG	1:62:A:ASN:H	10	0.66
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	10	0.66
(1,1738)	1:176:A:HIS:HD2	1:135:A:TYR:H	1	0.66
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD11	7	0.66
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD12	7	0.66
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD13	7	0.66
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD11	7	0.66
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD12	7	0.66
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD13	7	0.66
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD11	7	0.66
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD12	7	0.66
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD13	7	0.66
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	5	0.66
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	5	0.66
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	5	0.66
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	8	0.66
(1,1557)	1:140:A:GLU:HB2	1:169:A:GLN:HE22	9	0.66
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	2	0.66
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	2	0.66
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD1	8	0.66
(1,1087)	1:120:A:PHE:H	1:135:A:TYR:HD2	8	0.66
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	6	0.66
(1,955)	1:38:A:LEU:HB3	1:41:A:ILE:HD11	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:38:A:LEU:HB3	1:41:A:ILE:HD12	7	0.66
(1,955)	1:38:A:LEU:HB3	1:41:A:ILE:HD13	7	0.66
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	4	0.66
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	4	0.66
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	4	0.66
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	5	0.66
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	5	0.66
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	5	0.66
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	1	0.66
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	10	0.66
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	6	0.66
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	6	0.66
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	6	0.66
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	8	0.66
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	5	0.65
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	5	0.65
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	5	0.65
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	8	0.65
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	8	0.65
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	8	0.65
(1,3311)	1:158:A:HIS:HD2	1:157:A:ILE:HG12	10	0.65
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	4	0.65
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	4	0.65
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	4	0.65
(1,3193)	1:66:A:ILE:HG12	1:63:A:ALA:H	9	0.65
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	9	0.65
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	9	0.65
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	9	0.65
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	5	0.65
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	5	0.65
(1,2871)	1:181:A:ILE:H	1:130:A:GLY:H	7	0.65
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD21	4	0.65
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD22	4	0.65
(1,2866)	1:28:A:GLU:H	1:51:A:LEU:HD23	4	0.65
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG11	5	0.65
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG12	5	0.65
(1,2806)	1:157:A:ILE:HB	1:94:A:VAL:HG13	5	0.65
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	9	0.65
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG21	10	0.65
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG22	10	0.65
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG23	10	0.65
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG21	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG22	10	0.65
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG23	10	0.65
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG21	10	0.65
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG22	10	0.65
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG23	10	0.65
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB2	3	0.65
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB3	3	0.65
(1,2238)	1:130:A:GLY:HA3	1:125:A:ALA:HB1	3	0.65
(1,2238)	1:130:A:GLY:HA3	1:125:A:ALA:HB2	3	0.65
(1,2238)	1:130:A:GLY:HA3	1:125:A:ALA:HB3	3	0.65
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD21	4	0.65
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD22	4	0.65
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD23	4	0.65
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD21	4	0.65
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD22	4	0.65
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD23	4	0.65
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD21	4	0.65
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD22	4	0.65
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD23	4	0.65
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	1	0.65
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	5	0.65
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	10	0.65
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	3	0.65
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE1	8	0.65
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE2	8	0.65
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	7	0.65
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	5	0.65
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	10	0.65
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	6	0.65
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	1	0.65
(1,1558)	1:9:A:LEU:HA	1:11:A:LEU:HB2	9	0.65
(1,1509)	1:176:A:HIS:H	1:170:A:ARG:H	5	0.65
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	1	0.65
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	10	0.65
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	10	0.65
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	10	0.65
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	2	0.65
(1,864)	1:166:A:VAL:HB	1:178:A:GLN:H	10	0.65
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG21	7	0.65
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG22	7	0.65
(1,750)	1:183:A:GLU:HG2	1:160:A:THR:HG23	7	0.65
(1,574)	1:120:A:PHE:H	1:121:A:ARG:HB3	2	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:176:A:HIS:H	1:170:A:ARG:HA	9	0.65
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	1	0.65
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	1	0.65
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	9	0.65
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	9	0.65
(1,212)	1:162:A:ILE:HG21	1:182:A:GLU:H	7	0.65
(1,212)	1:162:A:ILE:HG22	1:182:A:GLU:H	7	0.65
(1,212)	1:162:A:ILE:HG23	1:182:A:GLU:H	7	0.65
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	7	0.64
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	7	0.64
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	7	0.64
(1,3384)	1:120:A:PHE:HD1	1:135:A:TYR:H	6	0.64
(1,3384)	1:120:A:PHE:HD2	1:135:A:TYR:H	6	0.64
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	1	0.64
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	1	0.64
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	1	0.64
(1,3073)	1:37:A:PHE:HA	1:6:A:ASN:H	1	0.64
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	7	0.64
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	7	0.64
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	7	0.64
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	10	0.64
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	10	0.64
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	10	0.64
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	2	0.64
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	5	0.64
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	5	0.64
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	5	0.64
(1,2424)	1:96:A:GLU:HB3	1:93:A:ASN:H	4	0.64
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	2	0.64
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	2	0.64
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	2	0.64
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	9	0.64
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	9	0.64
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	9	0.64
(1,2254)	1:157:A:ILE:HB	1:160:A:THR:H	6	0.64
(1,2011)	1:30:A:GLN:HE22	1:30:A:GLN:HA	2	0.64
(1,1750)	1:165:A:LYS:HB2	1:147:A:ILE:HG21	1	0.64
(1,1750)	1:165:A:LYS:HB2	1:147:A:ILE:HG22	1	0.64
(1,1750)	1:165:A:LYS:HB2	1:147:A:ILE:HG23	1	0.64
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	3	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	7	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	7	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	7	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	8	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	8	0.64
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	8	0.64
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	9	0.64
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	9	0.64
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	9	0.64
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	9	0.64
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	9	0.64
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	9	0.64
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	9	0.64
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	9	0.64
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	9	0.64
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	9	0.64
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	9	0.64
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	9	0.64
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	9	0.64
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	9	0.64
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	9	0.64
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	9	0.64
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	9	0.64
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	9	0.64
(1,1533)	1:161:A:GLU:HA	1:184:A:LYS:H	5	0.64
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG11	5	0.64
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG12	5	0.64
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG13	5	0.64
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG11	5	0.64
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG12	5	0.64
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG13	5	0.64
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG11	5	0.64
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG12	5	0.64
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG13	5	0.64
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	6	0.64
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	6	0.64
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	6	0.64
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	6	0.64
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	4	0.64
(1,316)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	8	0.64
(1,316)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	8	0.64
(1,316)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	8	0.64
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	6	0.64
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:101:A:LEU:HD21	2:201:A:Z90:HAM	2	0.64
(1,264)	1:101:A:LEU:HD22	2:201:A:Z90:HAM	2	0.64
(1,264)	1:101:A:LEU:HD23	2:201:A:Z90:HAM	2	0.64
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	3	0.64
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	3	0.64
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	3	0.64
(1,123)	1:30:A:GLN:HB3	1:32:A:ASP:H	8	0.64
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	10	0.63
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	6	0.63
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	6	0.63
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	6	0.63
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD21	7	0.63
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD22	7	0.63
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD23	7	0.63
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD1	7	0.63
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD2	7	0.63
(1,3048)	1:75:A:PHE:H	1:152:A:THR:HG21	8	0.63
(1,3048)	1:75:A:PHE:H	1:152:A:THR:HG22	8	0.63
(1,3048)	1:75:A:PHE:H	1:152:A:THR:HG23	8	0.63
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	7	0.63
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	2	0.63
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	2	0.63
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	2	0.63
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	1	0.63
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	1	0.63
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	1	0.63
(1,2577)	1:128:A:GLY:HA3	1:130:A:GLY:H	6	0.63
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	2	0.63
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	2	0.63
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	2	0.63
(1,2415)	1:75:A:PHE:HE1	1:156:A:GLN:H	5	0.63
(1,2415)	1:75:A:PHE:HE2	1:156:A:GLN:H	5	0.63
(1,2394)	1:17:A:TYR:HE1	1:13:A:VAL:H	7	0.63
(1,2394)	1:17:A:TYR:HE2	1:13:A:VAL:H	7	0.63
(1,2393)	1:14:A:ILE:HG12	1:13:A:VAL:H	2	0.63
(1,2340)	1:139:A:ARG:HG2	1:141:A:GLY:H	10	0.63
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	3	0.63
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	3	0.63
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	3	0.63
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	8	0.63
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG21	3	0.63
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG22	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG23	3	0.63
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG21	9	0.63
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG22	9	0.63
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG23	9	0.63
(1,1960)	1:184:A:LYS:HE2	1:184:A:LYS:HA	3	0.63
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	6	0.63
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	9	0.63
(1,1730)	1:25:A:ILE:HA	1:58:A:VAL:H	8	0.63
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	4	0.63
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE1	4	0.63
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE2	4	0.63
(1,1607)	1:8:A:ALA:HB1	1:73:A:MET:HE3	4	0.63
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE1	4	0.63
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE2	4	0.63
(1,1607)	1:8:A:ALA:HB2	1:73:A:MET:HE3	4	0.63
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE1	4	0.63
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE2	4	0.63
(1,1607)	1:8:A:ALA:HB3	1:73:A:MET:HE3	4	0.63
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	2	0.63
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	2	0.63
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	2	0.63
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	2	0.63
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	3	0.63
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG21	9	0.63
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG22	9	0.63
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG23	9	0.63
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	4	0.63
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	4	0.63
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	4	0.63
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	3	0.63
(1,311)	1:39:A:VAL:HG11	2:201:A:Z90:HAE	9	0.63
(1,311)	1:39:A:VAL:HG12	2:201:A:Z90:HAE	9	0.63
(1,311)	1:39:A:VAL:HG13	2:201:A:Z90:HAE	9	0.63
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	5	0.63
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	5	0.63
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	8	0.63
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	8	0.63
(1,301)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	3	0.63
(1,301)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	10	0.63
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	3	0.63
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	3	0.63
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	10	0.63
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	9	0.63
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	9	0.63
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	9	0.63
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	9	0.63
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	9	0.63
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	9	0.63
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD21	8	0.63
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD22	8	0.63
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD23	8	0.63
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	2	0.63
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	2	0.63
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	2	0.63
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	8	0.63
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	8	0.63
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	8	0.63
(1,198)	1:135:A:TYR:HE1	1:135:A:TYR:H	2	0.63
(1,198)	1:135:A:TYR:HE2	1:135:A:TYR:H	2	0.63
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG11	5	0.62
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG12	5	0.62
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG13	5	0.62
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG21	8	0.62
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG22	8	0.62
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG23	8	0.62
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	6	0.62
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	6	0.62
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	6	0.62
(1,2273)	1:11:A:LEU:HB3	1:8:A:ALA:H	8	0.62
(1,2188)	1:183:A:GLU:HB2	1:185:A:GLU:H	1	0.62
(1,1992)	1:92:A:SER:HB2	1:93:A:ASN:HD22	9	0.62
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	7	0.62
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	7	0.62
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	7	0.62
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE1	6	0.62
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE2	6	0.62
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE3	6	0.62
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	9	0.62
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	9	0.62
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	9	0.62
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	6	0.62
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	6	0.62
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD11	8	0.62
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD12	8	0.62
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD13	8	0.62
(1,1319)	1:167:A:ILE:HD11	1:133:A:LEU:H	1	0.62
(1,1319)	1:167:A:ILE:HD12	1:133:A:LEU:H	1	0.62
(1,1319)	1:167:A:ILE:HD13	1:133:A:LEU:H	1	0.62
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	10	0.62
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	8	0.62
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	8	0.62
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	8	0.62
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	3	0.62
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	3	0.62
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	3	0.62
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	2	0.62
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	2	0.62
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	2	0.62
(1,524)	1:124:A:ASP:HB2	1:131:A:LEU:H	10	0.62
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	1	0.62
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	1	0.62
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	1	0.62
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	1	0.62
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	1	0.62
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	1	0.62
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	10	0.62
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	10	0.62
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	10	0.62
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	2	0.62
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	2	0.62
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	2	0.62
(1,307)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	2	0.62
(1,307)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	2	0.62
(1,307)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	2	0.62
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	2	0.62
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	2	0.62
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	7	0.62
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	7	0.62
(1,301)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	2	0.62
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD21	9	0.62
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD22	9	0.62
(1,227)	1:63:A:ALA:H	1:67:A:LEU:HD23	9	0.62
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	4	0.62
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	4	0.62
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	4	0.62
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	4	0.62
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	4	0.62
(1,3391)	1:125:A:ALA:HA	1:128:A:GLY:H	1	0.61
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	9	0.61
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	9	0.61
(1,2935)	1:41:A:ILE:HG13	1:38:A:LEU:H	8	0.61
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE1	2	0.61
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE2	2	0.61
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE3	2	0.61
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD1	7	0.61
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD2	7	0.61
(1,2672)	1:179:A:PHE:HE1	1:146:A:VAL:H	1	0.61
(1,2672)	1:179:A:PHE:HE2	1:146:A:VAL:H	1	0.61
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	1	0.61
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	3	0.61
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	4	0.61
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	6	0.61
(1,2552)	1:99:A:GLN:HE22	1:96:A:GLU:H	1	0.61
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	10	0.61
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	10	0.61
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	10	0.61
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE1	6	0.61
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE2	6	0.61
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	2	0.61
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	2	0.61
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	2	0.61
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG21	5	0.61
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG22	5	0.61
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG23	5	0.61
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG21	10	0.61
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG22	10	0.61
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG23	10	0.61
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	3	0.61
(1,1810)	1:93:A:ASN:HD22	1:96:A:GLU:HB3	2	0.61
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	1	0.61
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	3	0.61
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	5	0.61
(1,1277)	1:100:A:ASN:HD22	1:103:A:ALA:H	8	0.61
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD11	10	0.61
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD12	10	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD13	10	0.61
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	6	0.61
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	6	0.61
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	6	0.61
(1,645)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	2	0.61
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	9	0.61
(1,479)	1:42:A:ILE:HA	1:3:A:GLY:H	6	0.61
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	9	0.61
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	9	0.61
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	9	0.61
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	9	0.61
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	9	0.61
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	9	0.61
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	10	0.61
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	10	0.61
(1,301)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	6	0.61
(1,274)	1:150:A:ILE:HG21	2:201:A:Z90:HAH	3	0.61
(1,274)	1:150:A:ILE:HG22	2:201:A:Z90:HAH	3	0.61
(1,274)	1:150:A:ILE:HG23	2:201:A:Z90:HAH	3	0.61
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	6	0.61
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	6	0.61
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	6	0.61
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD11	1	0.61
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD12	1	0.61
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD13	1	0.61
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	4	0.6
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	3	0.6
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	3	0.6
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	3	0.6
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	3	0.6
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	3	0.6
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	3	0.6
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	3	0.6
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	3	0.6
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	3	0.6
(1,3123)	1:23:A:GLU:HG3	1:22:A:TRP:H	1	0.6
(1,3113)	1:115:A:MET:HB2	1:117:A:ALA:H	1	0.6
(1,2992)	1:133:A:LEU:HG	1:123:A:THR:H	10	0.6
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD21	4	0.6
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD22	4	0.6
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD23	4	0.6
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD21	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD22	7	0.6
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD23	7	0.6
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	2	0.6
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	2	0.6
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	2	0.6
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	10	0.6
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	2	0.6
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	5	0.6
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	7	0.6
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	8	0.6
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	9	0.6
(1,2601)	1:31:A:LEU:HB3	1:31:A:LEU:HB2	10	0.6
(1,2466)	1:95:A:ARG:H	1:93:A:ASN:H	2	0.6
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	2	0.6
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	2	0.6
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	2	0.6
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD21	8	0.6
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD22	8	0.6
(1,2343)	1:48:A:THR:HB	1:9:A:LEU:HD23	8	0.6
(1,2316)	1:171:A:ASN:HB2	1:174:A:CYS:HB3	8	0.6
(1,2063)	1:93:A:ASN:HD22	1:93:A:ASN:H	3	0.6
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG21	10	0.6
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG22	10	0.6
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG23	10	0.6
(1,1997)	1:173:A:GLU:H	1:171:A:ASN:HA	8	0.6
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD2	2	0.6
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD3	2	0.6
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	8	0.6
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	8	0.6
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	8	0.6
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	7	0.6
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	3	0.6
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	3	0.6
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	3	0.6
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	6	0.6
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	9	0.6
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	9	0.6
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	9	0.6
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	7	0.6
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	6	0.6
(1,1053)	1:162:A:ILE:HA	1:164:A:MET:H	6	0.6
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	9	0.6
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	9	0.6
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG21	6	0.6
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG22	6	0.6
(1,776)	1:23:A:GLU:H	1:21:A:VAL:HG23	6	0.6
(1,626)	1:177:A:THR:HB	1:170:A:ARG:H	5	0.6
(1,624)	1:92:A:SER:H	1:96:A:GLU:HG3	9	0.6
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD11	10	0.6
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD12	10	0.6
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD13	10	0.6
(1,334)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	5	0.6
(1,334)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	5	0.6
(1,334)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	5	0.6
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	3	0.6
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	3	0.6
(1,303)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	4	0.6
(1,303)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	4	0.6
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	5	0.6
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	5	0.6
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	5	0.6
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	5	0.6
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	5	0.6
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	5	0.6
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	1	0.59
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	1	0.59
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	1	0.59
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD21	1	0.59
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD22	1	0.59
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD23	1	0.59
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD21	1	0.59
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD22	1	0.59
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD23	1	0.59
(1,3133)	1:60:A:ASN:HD22	1:60:A:ASN:H	1	0.59
(1,3108)	1:99:A:GLN:HE22	1:99:A:GLN:H	4	0.59
(1,2949)	1:58:A:VAL:HG11	1:21:A:VAL:H	3	0.59
(1,2949)	1:58:A:VAL:HG12	1:21:A:VAL:H	3	0.59
(1,2949)	1:58:A:VAL:HG13	1:21:A:VAL:H	3	0.59
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	6	0.59
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	6	0.59
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	6	0.59
(1,2884)	1:131:A:LEU:HB3	1:130:A:GLY:H	2	0.59
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	6	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	6	0.59
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	6	0.59
(1,2771)	1:137:A:SER:HA	1:119:A:SER:H	1	0.59
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	8	0.59
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	8	0.59
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	8	0.59
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	5	0.59
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	5	0.59
(1,2425)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	5	0.59
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	10	0.59
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	10	0.59
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	10	0.59
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	8	0.59
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	8	0.59
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	8	0.59
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	6	0.59
(1,1870)	1:92:A:SER:H	1:93:A:ASN:HA	5	0.59
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	9	0.59
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	8	0.59
(1,1617)	1:49:A:TYR:HE1	1:48:A:THR:H	4	0.59
(1,1617)	1:49:A:TYR:HE2	1:48:A:THR:H	4	0.59
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	9	0.59
(1,1459)	1:79:A:GLN:HB2	1:82:A:GLY:H	4	0.59
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD21	1	0.59
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD22	1	0.59
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD23	1	0.59
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	3	0.59
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	3	0.59
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	3	0.59
(1,1156)	1:100:A:ASN:HB3	1:99:A:GLN:H	3	0.59
(1,1138)	1:73:A:MET:HE1	1:16:A:ASN:H	8	0.59
(1,1138)	1:73:A:MET:HE2	1:16:A:ASN:H	8	0.59
(1,1138)	1:73:A:MET:HE3	1:16:A:ASN:H	8	0.59
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	8	0.59
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	4	0.59
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	9	0.59
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	9	0.59
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	9	0.59
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	9	0.59
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	9	0.59
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	9	0.59
(1,82)	1:19:A:PRO:HG2	1:21:A:VAL:H	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:19:A:PRO:HG3	1:21:A:VAL:H	8	0.59
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG21	4	0.59
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG22	4	0.59
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG23	4	0.59
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG21	4	0.59
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG22	4	0.59
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG23	4	0.59
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG21	4	0.59
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG22	4	0.59
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG23	4	0.59
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG21	6	0.59
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG22	6	0.59
(1,42)	1:121:A:ARG:HG2	1:132:A:ILE:HG23	6	0.59
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG21	6	0.59
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG22	6	0.59
(1,42)	1:121:A:ARG:HG3	1:132:A:ILE:HG23	6	0.59
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	7	0.58
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	7	0.58
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	7	0.58
(1,3436)	1:34:A:GLU:H	1:35:A:GLY:H	9	0.58
(1,3384)	1:120:A:PHE:HD1	1:135:A:TYR:H	3	0.58
(1,3384)	1:120:A:PHE:HD2	1:135:A:TYR:H	3	0.58
(1,3185)	1:16:A:ASN:HD22	1:16:A:ASN:H	5	0.58
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	3	0.58
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	3	0.58
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	3	0.58
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	5	0.58
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	6	0.58
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG21	9	0.58
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG22	9	0.58
(1,2652)	1:165:A:LYS:HB3	1:166:A:VAL:HG23	9	0.58
(1,2624)	1:173:A:GLU:HG2	1:172:A:GLU:H	10	0.58
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	2	0.58
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	2	0.58
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	2	0.58
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD21	10	0.58
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD22	10	0.58
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD23	10	0.58
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	7	0.58
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB2	6	0.58
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB3	6	0.58
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	10	0.58
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	10	0.58
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	8	0.58
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	8	0.58
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	8	0.58
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	9	0.58
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	9	0.58
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	9	0.58
(1,2011)	1:30:A:GLN:HE22	1:30:A:GLN:HA	10	0.58
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	6	0.58
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	6	0.58
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	6	0.58
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	5	0.58
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	4	0.58
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	8	0.58
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	4	0.58
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	4	0.58
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	4	0.58
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	4	0.58
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	4	0.58
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	4	0.58
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	4	0.58
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	4	0.58
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	4	0.58
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	4	0.58
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	4	0.58
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	4	0.58
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	4	0.58
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	4	0.58
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	4	0.58
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	4	0.58
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	4	0.58
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	4	0.58
(1,1480)	1:171:A:ASN:HD22	1:171:A:ASN:HA	6	0.58
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	5	0.58
(1,1131)	1:46:A:SER:H	1:44:A:ASP:HB3	5	0.58
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	10	0.58
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	5	0.58
(1,935)	1:125:A:ALA:HA	1:132:A:ILE:HB	10	0.58
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	7	0.58
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	7	0.58
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,767)	1:66:A:ILE:HG12	1:61:A:LEU:H	10	0.58
(1,764)	1:59:A:LEU:HD11	1:66:A:ILE:HD11	2	0.58
(1,764)	1:59:A:LEU:HD11	1:66:A:ILE:HD12	2	0.58
(1,764)	1:59:A:LEU:HD11	1:66:A:ILE:HD13	2	0.58
(1,764)	1:59:A:LEU:HD12	1:66:A:ILE:HD11	2	0.58
(1,764)	1:59:A:LEU:HD12	1:66:A:ILE:HD12	2	0.58
(1,764)	1:59:A:LEU:HD12	1:66:A:ILE:HD13	2	0.58
(1,764)	1:59:A:LEU:HD13	1:66:A:ILE:HD11	2	0.58
(1,764)	1:59:A:LEU:HD13	1:66:A:ILE:HD12	2	0.58
(1,764)	1:59:A:LEU:HD13	1:66:A:ILE:HD13	2	0.58
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG11	1	0.58
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG12	1	0.58
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG13	1	0.58
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	7	0.58
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	7	0.58
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	7	0.58
(1,401)	1:132:A:ILE:HA	1:125:A:ALA:H	7	0.58
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD11	9	0.58
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD12	9	0.58
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD13	9	0.58
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	6	0.58
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	6	0.58
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	6	0.58
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	2	0.58
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	2	0.58
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	2	0.58
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	9	0.58
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	9	0.58
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	9	0.58
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	9	0.58
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	9	0.58
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	9	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	1	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	1	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	1	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	1	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	1	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	1	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	6	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	6	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	6	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	6	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	6	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	6	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	10	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	10	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	10	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	10	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	10	0.58
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	10	0.58
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	9	0.57
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD11	8	0.57
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD12	8	0.57
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD13	8	0.57
(1,3354)	1:27:A:LYS:HD3	1:28:A:GLU:H	5	0.57
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG21	3	0.57
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG22	3	0.57
(1,3243)	1:9:A:LEU:H	1:48:A:THR:HG23	3	0.57
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	10	0.57
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	10	0.57
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	10	0.57
(1,2701)	1:99:A:GLN:HE22	1:95:A:ARG:HG3	9	0.57
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG21	7	0.57
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG22	7	0.57
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG23	7	0.57
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	8	0.57
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	8	0.57
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	8	0.57
(1,2219)	1:183:A:GLU:HG2	1:184:A:LYS:H	8	0.57
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	5	0.57
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	3	0.57
(1,1935)	1:135:A:TYR:HD1	1:119:A:SER:H	4	0.57
(1,1935)	1:135:A:TYR:HD2	1:119:A:SER:H	4	0.57
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	3	0.57
(1,1810)	1:93:A:ASN:HD22	1:96:A:GLU:HB3	10	0.57
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	2	0.57
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	10	0.57
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	8	0.57
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	7	0.57
(1,1470)	1:133:A:LEU:HA	1:133:A:LEU:HD21	10	0.57
(1,1470)	1:133:A:LEU:HA	1:133:A:LEU:HD22	10	0.57
(1,1470)	1:133:A:LEU:HA	1:133:A:LEU:HD23	10	0.57
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	3	0.57
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	9	0.57
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	9	0.57
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	9	0.57
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	10	0.57
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	10	0.57
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	10	0.57
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	3	0.57
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	9	0.57
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	1	0.57
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	1	0.57
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	1	0.57
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	2	0.57
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	9	0.57
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	9	0.57
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	9	0.57
(1,318)	1:101:A:LEU:HD21	2:201:A:Z90:HAM	1	0.57
(1,318)	1:101:A:LEU:HD22	2:201:A:Z90:HAM	1	0.57
(1,318)	1:101:A:LEU:HD23	2:201:A:Z90:HAM	1	0.57
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	10	0.57
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	10	0.57
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	10	0.57
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	10	0.57
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	10	0.57
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	10	0.57
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	10	0.57
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	10	0.57
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	10	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	3	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	3	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	3	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	3	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	3	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	3	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	4	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	4	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	4	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	4	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	4	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	4	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	5	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	5	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	5	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	5	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	5	0.57
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	5	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	2	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	2	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	2	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	2	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	2	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	2	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	7	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	7	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	7	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	7	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	7	0.57
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	7	0.57
(2,4)	1:139:A:ARG:HH21	2:201:A:Z90:OAB	3	0.56
(1,3484)	1:37:A:PHE:H	1:35:A:GLY:H	3	0.56
(1,3436)	1:34:A:GLU:H	1:35:A:GLY:H	7	0.56
(1,3205)	1:120:A:PHE:HD1	1:119:A:SER:H	10	0.56
(1,3205)	1:120:A:PHE:HD2	1:119:A:SER:H	10	0.56
(1,2951)	1:36:A:GLN:H	1:35:A:GLY:H	8	0.56
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD1	2	0.56
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD2	2	0.56
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	2	0.56
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	2	0.56
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	2	0.56
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	10	0.56
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	10	0.56
(1,2424)	1:96:A:GLU:HB3	1:93:A:ASN:H	9	0.56
(1,2198)	1:37:A:PHE:HD1	1:6:A:ASN:H	9	0.56
(1,2198)	1:37:A:PHE:HD2	1:6:A:ASN:H	9	0.56
(1,2118)	1:94:A:VAL:HG21	1:96:A:GLU:H	4	0.56
(1,2118)	1:94:A:VAL:HG22	1:96:A:GLU:H	4	0.56
(1,2118)	1:94:A:VAL:HG23	1:96:A:GLU:H	4	0.56
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	9	0.56
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	9	0.56
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	9	0.56
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	8	0.56
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	8	0.56
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	8	0.56
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	8	0.56
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	8	0.56
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	8	0.56
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	8	0.56
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	8	0.56
(1,1279)	1:30:A:GLN:HE22	1:29:A:ALA:H	9	0.56
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	2	0.56
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	2	0.56
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	2	0.56
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	2	0.56
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	2	0.56
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	2	0.56
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	2	0.56
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	2	0.56
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	2	0.56
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	6	0.56
(1,892)	1:172:A:GLU:H	1:171:A:ASN:HD22	4	0.56
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	5	0.56
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	5	0.56
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	5	0.56
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	1	0.56
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	1	0.56
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	1	0.56
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	5	0.56
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	7	0.56
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	7	0.56
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	7	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD11	4	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD12	4	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD13	4	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD11	5	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD12	5	0.56
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD13	5	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	7	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	7	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	7	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	7	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	7	0.56
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	7	0.56
(1,313)	1:39:A:VAL:HG21	2:201:A:Z90:HAE	7	0.56
(1,313)	1:39:A:VAL:HG22	2:201:A:Z90:HAE	7	0.56
(1,313)	1:39:A:VAL:HG23	2:201:A:Z90:HAE	7	0.56
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	5	0.56
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	5	0.56
(1,289)	1:149:A:ILE:HG21	2:201:A:Z90:HAI	8	0.56
(1,289)	1:149:A:ILE:HG22	2:201:A:Z90:HAI	8	0.56
(1,289)	1:149:A:ILE:HG23	2:201:A:Z90:HAI	8	0.56
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	1	0.56
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	1	0.56
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	9	0.56
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	9	0.56
(1,277)	1:149:A:ILE:HG21	2:201:A:Z90:HAM	7	0.56
(1,277)	1:149:A:ILE:HG22	2:201:A:Z90:HAM	7	0.56
(1,277)	1:149:A:ILE:HG23	2:201:A:Z90:HAM	7	0.56
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	1	0.56
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	7	0.56
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	7	0.56
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	7	0.56
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	7	0.56
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	7	0.56
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	7	0.56
(1,212)	1:162:A:ILE:HG21	1:182:A:GLU:H	8	0.56
(1,212)	1:162:A:ILE:HG22	1:182:A:GLU:H	8	0.56
(1,212)	1:162:A:ILE:HG23	1:182:A:GLU:H	8	0.56
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB2	5	0.56
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB3	5	0.56
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG21	3	0.56
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG22	3	0.56
(1,49)	1:69:A:MET:HE1	1:66:A:ILE:HG23	3	0.56
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG21	3	0.56
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG22	3	0.56
(1,49)	1:69:A:MET:HE2	1:66:A:ILE:HG23	3	0.56
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG21	3	0.56
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG22	3	0.56
(1,49)	1:69:A:MET:HE3	1:66:A:ILE:HG23	3	0.56
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	9	0.56
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	9	0.56
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	9	0.56
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	9	0.56
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	9	0.56
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	9	0.56
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	10	0.55
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	10	0.55
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	10	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG21	10	0.55
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG22	10	0.55
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG23	10	0.55
(1,3024)	1:126:A:GLU:HG2	1:126:A:GLU:H	9	0.55
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	4	0.55
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD1	3	0.55
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD2	3	0.55
(1,2624)	1:173:A:GLU:HG2	1:172:A:GLU:H	5	0.55
(1,2327)	1:173:A:GLU:H	1:174:A:CYS:HB3	9	0.55
(1,2192)	1:65:A:GLU:HG2	1:63:A:ALA:H	6	0.55
(1,2192)	1:65:A:GLU:HG3	1:63:A:ALA:H	6	0.55
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	6	0.55
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	6	0.55
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	6	0.55
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD21	7	0.55
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD22	7	0.55
(1,1999)	1:10:A:GLU:HG2	1:9:A:LEU:HD23	7	0.55
(1,1867)	1:173:A:GLU:H	1:171:A:ASN:H	8	0.55
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	8	0.55
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	8	0.55
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	4	0.55
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	3	0.55
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	8	0.55
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	2	0.55
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD11	10	0.55
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD12	10	0.55
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD13	10	0.55
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD11	8	0.55
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD12	8	0.55
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD13	8	0.55
(1,1077)	1:184:A:LYS:HA	1:185:A:GLU:H	5	0.55
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE1	1	0.55
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE2	1	0.55
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE1	1	0.55
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE2	1	0.55
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE1	1	0.55
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE2	1	0.55
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD11	6	0.55
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD12	6	0.55
(1,950)	1:149:A:ILE:HD11	1:150:A:ILE:HD13	6	0.55
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD11	6	0.55
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD12	6	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:149:A:ILE:HD12	1:150:A:ILE:HD13	6	0.55
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD11	6	0.55
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD12	6	0.55
(1,950)	1:149:A:ILE:HD13	1:150:A:ILE:HD13	6	0.55
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	5	0.55
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	5	0.55
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	5	0.55
(1,728)	1:144:A:ASP:HB2	1:68:A:GLN:H	9	0.55
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	1	0.55
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD11	6	0.55
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD12	6	0.55
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD13	6	0.55
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	8	0.55
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	8	0.55
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	8	0.55
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	8	0.55
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	8	0.55
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	8	0.55
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	4	0.55
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	4	0.55
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	6	0.55
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	6	0.55
(1,264)	1:101:A:LEU:HD21	2:201:A:Z90:HAM	1	0.55
(1,264)	1:101:A:LEU:HD22	2:201:A:Z90:HAM	1	0.55
(1,264)	1:101:A:LEU:HD23	2:201:A:Z90:HAM	1	0.55
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	3	0.55
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	7	0.55
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD21	9	0.54
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD22	9	0.54
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD23	9	0.54
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD21	9	0.54
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD22	9	0.54
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD23	9	0.54
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD21	9	0.54
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD22	9	0.54
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD23	9	0.54
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	5	0.54
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	5	0.54
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	5	0.54
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	6	0.54
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	6	0.54
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	5	0.54
(1,2720)	1:140:A:GLU:HG2	1:142:A:LEU:H	10	0.54
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	3	0.54
(1,2198)	1:37:A:PHE:HD1	1:6:A:ASN:H	4	0.54
(1,2198)	1:37:A:PHE:HD2	1:6:A:ASN:H	4	0.54
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	8	0.54
(1,2025)	1:47:A:LYS:HE2	1:47:A:LYS:H	6	0.54
(1,2011)	1:30:A:GLN:HE22	1:30:A:GLN:HA	5	0.54
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	3	0.54
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	3	0.54
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	3	0.54
(1,1962)	1:184:A:LYS:HA	1:183:A:GLU:HG3	10	0.54
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB2	9	0.54
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB3	9	0.54
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	4	0.54
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	9	0.54
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD21	2	0.54
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD22	2	0.54
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD23	2	0.54
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	3	0.54
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	3	0.54
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	3	0.54
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	3	0.54
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	3	0.54
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	3	0.54
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	3	0.54
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	3	0.54
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	3	0.54
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	3	0.54
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	3	0.54
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	3	0.54
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	3	0.54
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	3	0.54
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	3	0.54
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	3	0.54
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	3	0.54
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	3	0.54
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	3	0.54
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	3	0.54
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	3	0.54
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	8	0.54
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	4	0.54
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	4	0.54
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	4	0.54
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	5	0.54
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD21	7	0.54
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD22	7	0.54
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD23	7	0.54
(1,892)	1:172:A:GLU:H	1:171:A:ASN:HD22	8	0.54
(1,870)	1:69:A:MET:HE1	1:59:A:LEU:HG	6	0.54
(1,870)	1:69:A:MET:HE2	1:59:A:LEU:HG	6	0.54
(1,870)	1:69:A:MET:HE3	1:59:A:LEU:HG	6	0.54
(1,794)	1:136:A:TYR:HD1	1:177:A:THR:H	8	0.54
(1,794)	1:136:A:TYR:HD2	1:177:A:THR:H	8	0.54
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	9	0.54
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	9	0.54
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	9	0.54
(1,645)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	8	0.54
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	7	0.54
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	1	0.54
(1,313)	1:39:A:VAL:HG21	2:201:A:Z90:HAE	5	0.54
(1,313)	1:39:A:VAL:HG22	2:201:A:Z90:HAE	5	0.54
(1,313)	1:39:A:VAL:HG23	2:201:A:Z90:HAE	5	0.54
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	1	0.54
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	1	0.54
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	1	0.54
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	5	0.54
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	9	0.54
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	9	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	1	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	1	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	3	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	3	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	6	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	6	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	7	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	7	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	8	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	8	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	10	0.54
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	10	0.54
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	2	0.54
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	5	0.54
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	5	0.54
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	8	0.54
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	8	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	2	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	2	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	2	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	2	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	2	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	2	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	4	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	4	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	4	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	4	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	4	0.54
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	4	0.54
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	10	0.54
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	10	0.54
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD11	8	0.54
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD12	8	0.54
(1,79)	1:55:A:ALA:HB1	1:51:A:LEU:HD13	8	0.54
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD11	8	0.54
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD12	8	0.54
(1,79)	1:55:A:ALA:HB2	1:51:A:LEU:HD13	8	0.54
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD11	8	0.54
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD12	8	0.54
(1,79)	1:55:A:ALA:HB3	1:51:A:LEU:HD13	8	0.54
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	8	0.53
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	9	0.53
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	9	0.53
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	9	0.53
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	9	0.53
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	6	0.53
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	6	0.53
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	6	0.53
(1,2531)	1:31:A:LEU:HD11	1:29:A:ALA:H	1	0.53
(1,2531)	1:31:A:LEU:HD12	1:29:A:ALA:H	1	0.53
(1,2531)	1:31:A:LEU:HD13	1:29:A:ALA:H	1	0.53
(1,2424)	1:96:A:GLU:HB3	1:93:A:ASN:H	1	0.53
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE1	10	0.53
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE2	10	0.53
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG21	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG22	5	0.53
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG23	5	0.53
(1,2042)	1:176:A:HIS:H	1:174:A:CYS:H	3	0.53
(1,1927)	1:120:A:PHE:HE1	1:119:A:SER:H	6	0.53
(1,1927)	1:120:A:PHE:HE2	1:119:A:SER:H	6	0.53
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB1	2	0.53
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB2	2	0.53
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB3	2	0.53
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG21	4	0.53
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG22	4	0.53
(1,1576)	1:146:A:VAL:H	1:147:A:ILE:HG23	4	0.53
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	3	0.53
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	3	0.53
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	3	0.53
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	3	0.53
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	3	0.53
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	3	0.53
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	3	0.53
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	3	0.53
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	3	0.53
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	3	0.53
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	8	0.53
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	10	0.53
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	10	0.53
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	10	0.53
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG21	6	0.53
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG22	6	0.53
(1,675)	1:156:A:GLN:HE22	1:152:A:THR:HG23	6	0.53
(1,358)	1:127:A:LYS:HD2	1:128:A:GLY:H	4	0.53
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	4	0.53
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	4	0.53
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	4	0.53
(1,305)	1:149:A:ILE:HG21	2:201:A:Z90:HAM	7	0.53
(1,305)	1:149:A:ILE:HG22	2:201:A:Z90:HAM	7	0.53
(1,305)	1:149:A:ILE:HG23	2:201:A:Z90:HAM	7	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	1	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	1	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	2	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	2	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	5	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	5	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	6	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	7	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	7	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	8	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	8	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	10	0.53
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	10	0.53
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	2	0.53
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	2	0.53
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	7	0.53
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	7	0.53
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	5	0.53
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	5	0.53
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	5	0.53
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG21	3	0.52
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG22	3	0.52
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG23	3	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG21	3	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG22	3	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG23	3	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG21	3	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG22	3	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG23	3	0.52
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG21	5	0.52
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG22	5	0.52
(1,3412)	1:150:A:ILE:HG21	1:153:A:VAL:HG23	5	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG21	5	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG22	5	0.52
(1,3412)	1:150:A:ILE:HG22	1:153:A:VAL:HG23	5	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG21	5	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG22	5	0.52
(1,3412)	1:150:A:ILE:HG23	1:153:A:VAL:HG23	5	0.52
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD11	6	0.52
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD12	6	0.52
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD13	6	0.52
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD21	4	0.52
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD22	4	0.52
(1,3132)	1:41:A:ILE:HG13	1:38:A:LEU:HD23	4	0.52
(1,2961)	1:123:A:THR:HB	1:124:A:ASP:H	10	0.52
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD1	5	0.52
(1,2889)	1:135:A:TYR:HA	1:136:A:TYR:HD2	5	0.52
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2803)	1:155:A:GLN:HG2	1:159:A:GLY:H	3	0.52
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	5	0.52
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	5	0.52
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	5	0.52
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	5	0.52
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	5	0.52
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	5	0.52
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	5	0.52
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	5	0.52
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	5	0.52
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	10	0.52
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	10	0.52
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	10	0.52
(1,2273)	1:11:A:LEU:HB3	1:8:A:ALA:H	3	0.52
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	5	0.52
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	5	0.52
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	5	0.52
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB1	7	0.52
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB2	7	0.52
(1,2142)	1:30:A:GLN:HB3	1:29:A:ALA:HB3	7	0.52
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	10	0.52
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	7	0.52
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	7	0.52
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	7	0.52
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	4	0.52
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	4	0.52
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	4	0.52
(1,1156)	1:100:A:ASN:HB3	1:99:A:GLN:H	2	0.52
(1,1001)	1:183:A:GLU:HG3	1:184:A:LYS:H	5	0.52
(1,864)	1:166:A:VAL:HB	1:178:A:GLN:H	1	0.52
(1,548)	1:143:A:GLN:HE22	1:144:A:ASP:H	6	0.52
(1,525)	1:131:A:LEU:HB2	1:183:A:GLU:H	2	0.52
(1,401)	1:132:A:ILE:HA	1:125:A:ALA:H	3	0.52
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD11	1	0.52
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD12	1	0.52
(1,374)	1:11:A:LEU:HA	1:11:A:LEU:HD13	1	0.52
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	1	0.52
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	1	0.52
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	1	0.52
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	3	0.52
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	3	0.52
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	10	0.52
(1,265)	1:101:A:LEU:HD11	2:201:A:Z90:HAM	8	0.52
(1,265)	1:101:A:LEU:HD12	2:201:A:Z90:HAM	8	0.52
(1,265)	1:101:A:LEU:HD13	2:201:A:Z90:HAM	8	0.52
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	9	0.52
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	3	0.52
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD11	3	0.52
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD12	3	0.52
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD13	3	0.52
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD21	3	0.52
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD22	3	0.52
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD23	3	0.52
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD21	8	0.52
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD22	8	0.52
(1,76)	1:139:A:ARG:HG2	1:142:A:LEU:HD23	8	0.52
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD21	8	0.52
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD22	8	0.52
(1,76)	1:139:A:ARG:HG3	1:142:A:LEU:HD23	8	0.52
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	1	0.52
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	1	0.52
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	1	0.52
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	1	0.52
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	1	0.52
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	1	0.52
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	5	0.51
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	5	0.51
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	5	0.51
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	9	0.51
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	9	0.51
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	9	0.51
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	7	0.51
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	7	0.51
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	7	0.51
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	7	0.51
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	7	0.51
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	7	0.51
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	7	0.51
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	7	0.51
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	7	0.51
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG21	1	0.51
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG22	1	0.51
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG23	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD11	4	0.51
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD12	4	0.51
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD13	4	0.51
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	8	0.51
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	8	0.51
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	8	0.51
(1,2631)	1:21:A:VAL:HB	1:25:A:ILE:H	5	0.51
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	7	0.51
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	7	0.51
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	7	0.51
(1,2415)	1:75:A:PHE:HE1	1:156:A:GLN:H	6	0.51
(1,2415)	1:75:A:PHE:HE2	1:156:A:GLN:H	6	0.51
(1,2394)	1:17:A:TYR:HE1	1:13:A:VAL:H	6	0.51
(1,2394)	1:17:A:TYR:HE2	1:13:A:VAL:H	6	0.51
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	3	0.51
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	8	0.51
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	8	0.51
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	8	0.51
(1,2113)	1:62:A:ASN:HB2	1:61:A:LEU:HA	4	0.51
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	4	0.51
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	4	0.51
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	4	0.51
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	9	0.51
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD11	5	0.51
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD12	5	0.51
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD13	5	0.51
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD11	5	0.51
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD12	5	0.51
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD13	5	0.51
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD11	5	0.51
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD12	5	0.51
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD13	5	0.51
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	1	0.51
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	1	0.51
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	7	0.51
(1,1172)	1:135:A:TYR:HD1	1:177:A:THR:H	7	0.51
(1,1172)	1:135:A:TYR:HD2	1:177:A:THR:H	7	0.51
(1,864)	1:166:A:VAL:HB	1:178:A:GLN:H	4	0.51
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	4	0.51
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	4	0.51
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	4	0.51
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	3	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	3	0.51
(1,670)	1:143:A:GLN:HG3	1:142:A:LEU:H	4	0.51
(1,334)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	6	0.51
(1,334)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	6	0.51
(1,334)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	6	0.51
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAY	4	0.51
(1,290)	2:201:A:Z90:HAF	2:201:A:Z90:HAYA	4	0.51
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	5	0.51
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	5	0.51
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	9	0.51
(1,280)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	9	0.51
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	3	0.51
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	3	0.51
(1,278)	2:201:A:Z90:HAZ	2:201:A:Z90:HAN	4	0.51
(1,278)	2:201:A:Z90:HAZA	2:201:A:Z90:HAN	4	0.51
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	4	0.51
(1,109)	1:165:A:LYS:HG3	1:180:A:LEU:H	5	0.51
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	2	0.51
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	2	0.51
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	7	0.5
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG21	6	0.5
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG22	6	0.5
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG23	6	0.5
(1,3233)	1:141:A:GLY:HA2	1:140:A:GLU:H	7	0.5
(1,3108)	1:99:A:GLN:HE22	1:99:A:GLN:H	8	0.5
(1,3072)	1:165:A:LYS:HE2	1:165:A:LYS:H	7	0.5
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	9	0.5
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	9	0.5
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	9	0.5
(1,2794)	1:146:A:VAL:HB	1:150:A:ILE:HD11	5	0.5
(1,2794)	1:146:A:VAL:HB	1:150:A:ILE:HD12	5	0.5
(1,2794)	1:146:A:VAL:HB	1:150:A:ILE:HD13	5	0.5
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	8	0.5
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	8	0.5
(1,2790)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	8	0.5
(1,2743)	1:62:A:ASN:HD22	1:65:A:GLU:HB2	2	0.5
(1,2743)	1:62:A:ASN:HD22	1:65:A:GLU:HB3	2	0.5
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	5	0.5
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	5	0.5
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	5	0.5
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	7	0.5
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	7	0.5
(1,2700)	1:120:A:PHE:HA	1:134:A:HIS:H	2	0.5
(1,2662)	1:56:A:SER:HB3	1:61:A:LEU:H	9	0.5
(1,2394)	1:17:A:TYR:HE1	1:13:A:VAL:H	9	0.5
(1,2394)	1:17:A:TYR:HE2	1:13:A:VAL:H	9	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	1	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	1	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	1	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	2	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	2	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	2	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	3	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	3	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	3	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	4	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	4	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	4	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	5	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	5	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	5	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	6	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	6	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	6	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	7	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	7	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	7	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	9	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	9	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	9	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG21	10	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG22	10	0.5
(1,2186)	1:157:A:ILE:HB	1:157:A:ILE:HG23	10	0.5
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	7	0.5
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	7	0.5
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	7	0.5
(1,2063)	1:93:A:ASN:HD22	1:93:A:ASN:H	8	0.5
(1,1951)	1:184:A:LYS:HE3	1:184:A:LYS:HA	5	0.5
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	6	0.5
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	5	0.5
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	5	0.5
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	5	0.5
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	5	0.5
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD11	8	0.5
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD12	8	0.5
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD13	8	0.5
(1,1490)	1:84:A:ASP:H	1:82:A:GLY:H	4	0.5
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	4	0.5
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	10	0.5
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	10	0.5
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	10	0.5
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	10	0.5
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	10	0.5
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	10	0.5
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	10	0.5
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	10	0.5
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	10	0.5
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD21	6	0.5
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD22	6	0.5
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD23	6	0.5
(1,1177)	1:37:A:PHE:H	1:37:A:PHE:HD1	10	0.5
(1,1177)	1:37:A:PHE:H	1:37:A:PHE:HD2	10	0.5
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	9	0.5
(1,1038)	1:177:A:THR:HA	1:169:A:GLN:H	2	0.5
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	5	0.5
(1,832)	1:21:A:VAL:HG11	1:20:A:GLU:H	3	0.5
(1,832)	1:21:A:VAL:HG12	1:20:A:GLU:H	3	0.5
(1,832)	1:21:A:VAL:HG13	1:20:A:GLU:H	3	0.5
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	8	0.5
(1,564)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	10	0.5
(1,479)	1:42:A:ILE:HA	1:3:A:GLY:H	7	0.5
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	10	0.5
(1,257)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	2	0.5
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	1	0.5
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	1	0.5
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	1	0.5
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	1	0.5
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	1	0.5
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	1	0.5
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD11	10	0.5
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD12	10	0.5
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD13	10	0.5
(1,183)	1:3:A:GLY:H	1:43:A:TYR:HE1	7	0.5
(1,183)	1:3:A:GLY:H	1:43:A:TYR:HE2	7	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB2	9	0.5
(1,173)	1:171:A:ASN:HD22	1:174:A:CYS:HB3	9	0.5
(1,3479)	1:98:A:LEU:HD11	1:133:A:LEU:HD21	4	0.49
(1,3479)	1:98:A:LEU:HD11	1:133:A:LEU:HD22	4	0.49
(1,3479)	1:98:A:LEU:HD11	1:133:A:LEU:HD23	4	0.49
(1,3479)	1:98:A:LEU:HD12	1:133:A:LEU:HD21	4	0.49
(1,3479)	1:98:A:LEU:HD12	1:133:A:LEU:HD22	4	0.49
(1,3479)	1:98:A:LEU:HD12	1:133:A:LEU:HD23	4	0.49
(1,3479)	1:98:A:LEU:HD13	1:133:A:LEU:HD21	4	0.49
(1,3479)	1:98:A:LEU:HD13	1:133:A:LEU:HD22	4	0.49
(1,3479)	1:98:A:LEU:HD13	1:133:A:LEU:HD23	4	0.49
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD21	1	0.49
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD22	1	0.49
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD23	1	0.49
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG21	4	0.49
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG22	4	0.49
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG23	4	0.49
(1,3012)	1:176:A:HIS:H	1:174:A:CYS:HB3	2	0.49
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD21	9	0.49
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD22	9	0.49
(1,2851)	1:54:A:ALA:H	1:51:A:LEU:HD23	9	0.49
(1,2063)	1:93:A:ASN:HD22	1:93:A:ASN:H	7	0.49
(1,2042)	1:176:A:HIS:H	1:174:A:CYS:H	10	0.49
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	8	0.49
(1,1779)	1:171:A:ASN:HD22	1:173:A:GLU:HB2	5	0.49
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	3	0.49
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	6	0.49
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	9	0.49
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	2	0.49
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	8	0.49
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	8	0.49
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	8	0.49
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	8	0.49
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	8	0.49
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	8	0.49
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	8	0.49
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	8	0.49
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	8	0.49
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	8	0.49
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	8	0.49
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	8	0.49
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	8	0.49
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	8	0.49
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	8	0.49
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	8	0.49
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	8	0.49
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	8	0.49
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	5	0.49
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	2	0.49
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	8	0.49
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	3	0.49
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	3	0.49
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	3	0.49
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	1	0.49
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	2	0.49
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	10	0.49
(1,614)	1:170:A:ARG:HG2	1:170:A:ARG:H	3	0.49
(1,601)	1:170:A:ARG:HG2	1:171:A:ASN:H	10	0.49
(1,558)	1:125:A:ALA:HA	1:132:A:ILE:HG13	9	0.49
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	4	0.49
(1,525)	1:131:A:LEU:HB2	1:183:A:GLU:H	4	0.49
(1,335)	1:101:A:LEU:HD11	2:201:A:Z90:HAH	3	0.49
(1,335)	1:101:A:LEU:HD12	2:201:A:Z90:HAH	3	0.49
(1,335)	1:101:A:LEU:HD13	2:201:A:Z90:HAH	3	0.49
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD21	4	0.49
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD22	4	0.49
(1,315)	2:201:A:Z90:HAM	1:90:A:LEU:HD23	4	0.49
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	8	0.49
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	2	0.49
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	2	0.49
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	2	0.49
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	10	0.49
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	10	0.49
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	10	0.49
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	10	0.49
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	10	0.49
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	10	0.49
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	1	0.49
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	9	0.49
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	9	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	3	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	3	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	3	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	3	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	3	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	4	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	4	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	4	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	4	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	4	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	4	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	10	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	10	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	10	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	10	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	10	0.49
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	10	0.49
(3,5)	2:201:A:Z90:OAC	1:135:A:TYR:OH	7	0.48
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	1	0.48
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD21	3	0.48
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD22	3	0.48
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD23	3	0.48
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	4	0.48
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	4	0.48
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	4	0.48
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG21	3	0.48
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG22	3	0.48
(1,3371)	1:59:A:LEU:HA	1:58:A:VAL:HG23	3	0.48
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG21	2	0.48
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG22	2	0.48
(1,3191)	1:95:A:ARG:HD2	1:94:A:VAL:HG23	2	0.48
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG21	2	0.48
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG22	2	0.48
(1,3191)	1:95:A:ARG:HD3	1:94:A:VAL:HG23	2	0.48
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	3	0.48
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	9	0.48
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	9	0.48
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	9	0.48
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD11	7	0.48
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD12	7	0.48
(1,2918)	1:26:A:LYS:HE2	1:31:A:LEU:HD13	7	0.48
(1,2871)	1:181:A:ILE:H	1:130:A:GLY:H	9	0.48
(1,2863)	1:126:A:GLU:H	1:130:A:GLY:H	6	0.48
(1,2838)	1:132:A:ILE:HG13	1:133:A:LEU:H	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	9	0.48
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	8	0.48
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG21	3	0.48
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG22	3	0.48
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG23	3	0.48
(1,2634)	1:173:A:GLU:HG3	1:172:A:GLU:H	1	0.48
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG21	7	0.48
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG22	7	0.48
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG23	7	0.48
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG21	7	0.48
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG22	7	0.48
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG23	7	0.48
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG21	7	0.48
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG22	7	0.48
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG23	7	0.48
(1,2415)	1:75:A:PHE:HE1	1:156:A:GLN:H	10	0.48
(1,2415)	1:75:A:PHE:HE2	1:156:A:GLN:H	10	0.48
(1,2377)	1:133:A:LEU:HD21	1:122:A:CYS:H	8	0.48
(1,2377)	1:133:A:LEU:HD22	1:122:A:CYS:H	8	0.48
(1,2377)	1:133:A:LEU:HD23	1:122:A:CYS:H	8	0.48
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG21	2	0.48
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG22	2	0.48
(1,1976)	1:136:A:TYR:HD1	1:177:A:THR:HG23	2	0.48
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG21	2	0.48
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG22	2	0.48
(1,1976)	1:136:A:TYR:HD2	1:177:A:THR:HG23	2	0.48
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	10	0.48
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	9	0.48
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	9	0.48
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	9	0.48
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	10	0.48
(1,1820)	1:56:A:SER:HG	1:62:A:ASN:H	6	0.48
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	1	0.48
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD2	5	0.48
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD3	5	0.48
(1,1495)	1:125:A:ALA:HB1	1:131:A:LEU:H	8	0.48
(1,1495)	1:125:A:ALA:HB2	1:131:A:LEU:H	8	0.48
(1,1495)	1:125:A:ALA:HB3	1:131:A:LEU:H	8	0.48
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD11	2	0.48
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD12	2	0.48
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD13	2	0.48
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD11	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD12	2	0.48
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD13	2	0.48
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD11	2	0.48
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD12	2	0.48
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD13	2	0.48
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD11	9	0.48
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD12	9	0.48
(1,1280)	1:145:A:ILE:HG13	1:142:A:LEU:HD13	9	0.48
(1,1259)	1:184:A:LYS:HB3	1:161:A:GLU:H	1	0.48
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD21	8	0.48
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD22	8	0.48
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD23	8	0.48
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD21	9	0.48
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD22	9	0.48
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD23	9	0.48
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD11	1	0.48
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD12	1	0.48
(1,1221)	1:144:A:ASP:H	1:67:A:LEU:HD13	1	0.48
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	4	0.48
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	9	0.48
(1,892)	1:172:A:GLU:H	1:171:A:ASN:HD22	9	0.48
(1,810)	1:57:A:LYS:HG3	1:55:A:ALA:H	3	0.48
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	3	0.48
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	4	0.48
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	5	0.48
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	6	0.48
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	7	0.48
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	8	0.48
(1,683)	1:131:A:LEU:HB2	1:131:A:LEU:HB3	9	0.48
(1,462)	1:165:A:LYS:HD3	1:180:A:LEU:H	1	0.48
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	3	0.48
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG21	5	0.48
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG22	5	0.48
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG23	5	0.48
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB1	3	0.48
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB2	3	0.48
(1,331)	2:201:A:Z90:HAT	1:117:A:ALA:HB3	3	0.48
(1,277)	1:149:A:ILE:HG21	2:201:A:Z90:HAM	2	0.48
(1,277)	1:149:A:ILE:HG22	2:201:A:Z90:HAM	2	0.48
(1,277)	1:149:A:ILE:HG23	2:201:A:Z90:HAM	2	0.48
(1,261)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	6	0.48
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	9	0.48
(1,148)	1:145:A:ILE:HG12	1:143:A:GLN:H	7	0.48
(1,148)	1:145:A:ILE:HG13	1:143:A:GLN:H	7	0.48
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	2	0.48
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	2	0.48
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	8	0.48
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	8	0.48
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	8	0.48
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	8	0.48
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	8	0.48
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	8	0.48
(1,3540)	1:54:A:ALA:HB1	1:28:A:GLU:H	8	0.47
(1,3540)	1:54:A:ALA:HB2	1:28:A:GLU:H	8	0.47
(1,3540)	1:54:A:ALA:HB3	1:28:A:GLU:H	8	0.47
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD21	8	0.47
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD22	8	0.47
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD23	8	0.47
(1,3353)	1:91:A:GLY:H	1:93:A:ASN:H	8	0.47
(1,3072)	1:165:A:LYS:HE2	1:165:A:LYS:H	8	0.47
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	3	0.47
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	3	0.47
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD11	9	0.47
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD12	9	0.47
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD13	9	0.47
(1,1910)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	7	0.47
(1,1910)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	7	0.47
(1,1910)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	7	0.47
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	4	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	4	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	4	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	4	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	5	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	5	0.47
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	5	0.47
(1,1806)	1:183:A:GLU:HA	1:161:A:GLU:H	7	0.47
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	9	0.47
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	9	0.47
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG21	1	0.47
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG22	1	0.47
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG23	1	0.47
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG21	1	0.47
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG22	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG23	1	0.47
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	10	0.47
(1,1469)	1:171:A:ASN:HD22	1:171:A:ASN:HA	6	0.47
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG11	6	0.47
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG12	6	0.47
(1,1184)	2:201:A:Z90:HAM	1:153:A:VAL:HG13	6	0.47
(1,445)	1:95:A:ARG:HD2	1:95:A:ARG:HA	9	0.47
(1,445)	1:95:A:ARG:HD3	1:95:A:ARG:HA	9	0.47
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	7	0.47
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	7	0.47
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	7	0.47
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	8	0.47
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	8	0.47
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	8	0.47
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	9	0.47
(1,234)	1:157:A:ILE:HG13	1:159:A:GLY:H	10	0.47
(1,231)	1:145:A:ILE:HG21	1:144:A:ASP:H	2	0.47
(1,231)	1:145:A:ILE:HG22	1:144:A:ASP:H	2	0.47
(1,231)	1:145:A:ILE:HG23	1:144:A:ASP:H	2	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	5	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	5	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	5	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	5	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	5	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	5	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	7	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	7	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	7	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	7	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	7	0.47
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	7	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	5	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	5	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	5	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	5	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	5	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	5	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	6	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	6	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	6	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	6	0.47
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	6	0.47
(1,3526)	1:12:A:LEU:HA	1:16:A:ASN:HD22	1	0.46
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD21	1	0.46
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD22	1	0.46
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD23	1	0.46
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD11	10	0.46
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD12	10	0.46
(1,3389)	1:180:A:LEU:H	1:132:A:ILE:HD13	10	0.46
(1,3311)	1:158:A:HIS:HD2	1:157:A:ILE:HG12	2	0.46
(1,3108)	1:99:A:GLN:HE22	1:99:A:GLN:H	6	0.46
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG11	2	0.46
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG12	2	0.46
(1,2950)	1:158:A:HIS:HD2	1:94:A:VAL:HG13	2	0.46
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE1	10	0.46
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE2	10	0.46
(1,2907)	1:74:A:PHE:HA	1:73:A:MET:HE3	10	0.46
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	7	0.46
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	7	0.46
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	7	0.46
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	10	0.46
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	10	0.46
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	10	0.46
(1,2704)	1:62:A:ASN:HD22	1:61:A:LEU:HB2	4	0.46
(1,2577)	1:128:A:GLY:HA3	1:130:A:GLY:H	8	0.46
(1,2421)	1:72:A:LYS:H	1:148:A:GLY:H	8	0.46
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB1	6	0.46
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB2	6	0.46
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB3	6	0.46
(1,2125)	1:136:A:TYR:HA	1:119:A:SER:H	6	0.46
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG21	1	0.46
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG22	1	0.46
(1,2055)	1:24:A:ASP:HB3	1:21:A:VAL:HG23	1	0.46
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	7	0.46
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	9	0.46
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD21	5	0.46
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD22	5	0.46
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD23	5	0.46
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD21	5	0.46
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD22	5	0.46
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD23	5	0.46
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD21	5	0.46
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD22	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD23	5	0.46
(1,1951)	1:184:A:LYS:HE3	1:184:A:LYS:HA	9	0.46
(1,1944)	1:51:A:LEU:HD21	1:13:A:VAL:HG11	7	0.46
(1,1944)	1:51:A:LEU:HD21	1:13:A:VAL:HG12	7	0.46
(1,1944)	1:51:A:LEU:HD21	1:13:A:VAL:HG13	7	0.46
(1,1944)	1:51:A:LEU:HD21	1:13:A:VAL:HG21	7	0.46
(1,1944)	1:51:A:LEU:HD21	1:13:A:VAL:HG22	7	0.46
(1,1944)	1:51:A:LEU:HD21	1:13:A:VAL:HG23	7	0.46
(1,1944)	1:51:A:LEU:HD22	1:13:A:VAL:HG11	7	0.46
(1,1944)	1:51:A:LEU:HD22	1:13:A:VAL:HG12	7	0.46
(1,1944)	1:51:A:LEU:HD22	1:13:A:VAL:HG13	7	0.46
(1,1944)	1:51:A:LEU:HD22	1:13:A:VAL:HG21	7	0.46
(1,1944)	1:51:A:LEU:HD22	1:13:A:VAL:HG22	7	0.46
(1,1944)	1:51:A:LEU:HD22	1:13:A:VAL:HG23	7	0.46
(1,1944)	1:51:A:LEU:HD23	1:13:A:VAL:HG11	7	0.46
(1,1944)	1:51:A:LEU:HD23	1:13:A:VAL:HG12	7	0.46
(1,1944)	1:51:A:LEU:HD23	1:13:A:VAL:HG13	7	0.46
(1,1944)	1:51:A:LEU:HD23	1:13:A:VAL:HG21	7	0.46
(1,1944)	1:51:A:LEU:HD23	1:13:A:VAL:HG22	7	0.46
(1,1944)	1:51:A:LEU:HD23	1:13:A:VAL:HG23	7	0.46
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	6	0.46
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB2	8	0.46
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB3	8	0.46
(1,1733)	1:49:A:TYR:HD1	1:142:A:LEU:H	6	0.46
(1,1733)	1:49:A:TYR:HD2	1:142:A:LEU:H	6	0.46
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	2	0.46
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	2	0.46
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	2	0.46
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	2	0.46
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	2	0.46
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	2	0.46
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	2	0.46
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	2	0.46
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	2	0.46
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	2	0.46
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	2	0.46
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	2	0.46
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	2	0.46
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	2	0.46
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	2	0.46
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	2	0.46
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	2	0.46
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD21	7	0.46
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD22	7	0.46
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD23	7	0.46
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD11	9	0.46
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD12	9	0.46
(1,1320)	1:165:A:LYS:HE3	1:180:A:LEU:HD13	9	0.46
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	3	0.46
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	9	0.46
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE1	8	0.46
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE2	8	0.46
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE1	8	0.46
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE2	8	0.46
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE1	8	0.46
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE2	8	0.46
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD21	3	0.46
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD22	3	0.46
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD23	3	0.46
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD21	3	0.46
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD22	3	0.46
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD23	3	0.46
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD21	3	0.46
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD22	3	0.46
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD23	3	0.46
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	3	0.46
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	3	0.46
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	3	0.46
(1,622)	1:140:A:GLU:HB3	1:170:A:ARG:H	3	0.46
(1,522)	1:96:A:GLU:HG2	1:93:A:ASN:H	4	0.46
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG11	3	0.46
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG12	3	0.46
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG13	3	0.46
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	2	0.46
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	5	0.46
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	5	0.46
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	5	0.46
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	5	0.46
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	5	0.46
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	5	0.46
(1,148)	1:145:A:ILE:HG12	1:143:A:GLN:H	2	0.46
(1,148)	1:145:A:ILE:HG13	1:143:A:GLN:H	2	0.46
(1,120)	1:27:A:LYS:HD2	1:30:A:GLN:H	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:27:A:LYS:HD3	1:30:A:GLN:H	1	0.46
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	7	0.45
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	1	0.45
(1,3216)	1:27:A:LYS:HG2	1:27:A:LYS:H	4	0.45
(1,3044)	1:136:A:TYR:HD1	1:119:A:SER:H	2	0.45
(1,3044)	1:136:A:TYR:HD2	1:119:A:SER:H	2	0.45
(1,2961)	1:123:A:THR:HB	1:124:A:ASP:H	5	0.45
(1,2930)	1:61:A:LEU:HD11	1:66:A:ILE:H	3	0.45
(1,2930)	1:61:A:LEU:HD12	1:66:A:ILE:H	3	0.45
(1,2930)	1:61:A:LEU:HD13	1:66:A:ILE:H	3	0.45
(1,2930)	1:61:A:LEU:HD11	1:66:A:ILE:H	9	0.45
(1,2930)	1:61:A:LEU:HD12	1:66:A:ILE:H	9	0.45
(1,2930)	1:61:A:LEU:HD13	1:66:A:ILE:H	9	0.45
(1,2841)	1:65:A:GLU:HG2	1:65:A:GLU:H	6	0.45
(1,2841)	1:65:A:GLU:HG3	1:65:A:GLU:H	6	0.45
(1,2720)	1:140:A:GLU:HG2	1:142:A:LEU:H	8	0.45
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	1	0.45
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD21	2	0.45
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD22	2	0.45
(1,2593)	1:66:A:ILE:HG13	1:59:A:LEU:HD23	2	0.45
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG21	5	0.45
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG22	5	0.45
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG23	5	0.45
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG21	1	0.45
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG22	1	0.45
(1,2490)	1:123:A:THR:HG21	1:132:A:ILE:HG23	1	0.45
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG21	1	0.45
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG22	1	0.45
(1,2490)	1:123:A:THR:HG22	1:132:A:ILE:HG23	1	0.45
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG21	1	0.45
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG22	1	0.45
(1,2490)	1:123:A:THR:HG23	1:132:A:ILE:HG23	1	0.45
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG21	7	0.45
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG22	7	0.45
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG23	7	0.45
(1,2301)	1:136:A:TYR:HA	1:119:A:SER:H	6	0.45
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB1	1	0.45
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB2	1	0.45
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB3	1	0.45
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD21	8	0.45
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD22	8	0.45
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD23	8	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD21	8	0.45
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD22	8	0.45
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD23	8	0.45
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD21	8	0.45
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD22	8	0.45
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD23	8	0.45
(1,1956)	1:34:A:GLU:HB2	1:36:A:GLN:H	5	0.45
(1,1956)	1:34:A:GLU:HB3	1:36:A:GLN:H	5	0.45
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	1	0.45
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	1	0.45
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	1	0.45
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	1	0.45
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	6	0.45
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	7	0.45
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	7	0.45
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	4	0.45
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	4	0.45
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	4	0.45
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	10	0.45
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	10	0.45
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	10	0.45
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	3	0.45
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	3	0.45
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	3	0.45
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	3	0.45
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	3	0.45
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	3	0.45
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	3	0.45
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	3	0.45
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	3	0.45
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD21	5	0.45
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD22	5	0.45
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD23	5	0.45
(1,1050)	1:52:A:VAL:HG21	1:67:A:LEU:H	2	0.45
(1,1050)	1:52:A:VAL:HG22	1:67:A:LEU:H	2	0.45
(1,1050)	1:52:A:VAL:HG23	1:67:A:LEU:H	2	0.45
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD21	2	0.45
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD22	2	0.45
(1,914)	1:182:A:GLU:H	1:180:A:LEU:HD23	2	0.45
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	4	0.45
(1,649)	1:33:A:GLU:H	1:31:A:LEU:H	9	0.45
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE1	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE2	2	0.45
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE3	2	0.45
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD21	4	0.45
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD22	4	0.45
(1,508)	1:27:A:LYS:H	1:51:A:LEU:HD23	4	0.45
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	4	0.45
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	4	0.45
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	4	0.45
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	4	0.45
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	4	0.45
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	4	0.45
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD11	1	0.45
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD12	1	0.45
(1,322)	2:201:A:Z90:HAM	1:90:A:LEU:HD13	1	0.45
(1,305)	1:149:A:ILE:HG21	2:201:A:Z90:HAM	2	0.45
(1,305)	1:149:A:ILE:HG22	2:201:A:Z90:HAM	2	0.45
(1,305)	1:149:A:ILE:HG23	2:201:A:Z90:HAM	2	0.45
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	10	0.45
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD11	2	0.45
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD12	2	0.45
(1,212)	1:182:A:GLU:H	1:162:A:ILE:HD13	2	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	5	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	5	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	5	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	5	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	5	0.45
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	5	0.45
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	2	0.45
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	2	0.45
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	2	0.45
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD11	2	0.45
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD12	2	0.45
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD13	2	0.45
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	6	0.44
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	1	0.44
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	1	0.44
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	1	0.44
(1,3436)	1:34:A:GLU:H	1:35:A:GLY:H	3	0.44
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD11	9	0.44
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD12	9	0.44
(1,3261)	1:104:A:LEU:HD11	1:101:A:LEU:HD13	9	0.44
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD11	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD12	9	0.44
(1,3261)	1:104:A:LEU:HD12	1:101:A:LEU:HD13	9	0.44
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD11	9	0.44
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD12	9	0.44
(1,3261)	1:104:A:LEU:HD13	1:101:A:LEU:HD13	9	0.44
(1,3232)	1:32:A:ASP:HB3	1:27:A:LYS:H	5	0.44
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	8	0.44
(1,2936)	1:150:A:ILE:HD11	1:147:A:ILE:H	8	0.44
(1,2936)	1:150:A:ILE:HD12	1:147:A:ILE:H	8	0.44
(1,2936)	1:150:A:ILE:HD13	1:147:A:ILE:H	8	0.44
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	2	0.44
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	2	0.44
(1,2791)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	2	0.44
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	6	0.44
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	9	0.44
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	9	0.44
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	9	0.44
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB1	9	0.44
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB2	9	0.44
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB3	9	0.44
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD21	1	0.44
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD22	1	0.44
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD23	1	0.44
(1,2467)	1:125:A:ALA:H	1:130:A:GLY:H	6	0.44
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	5	0.44
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	5	0.44
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	5	0.44
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG21	8	0.44
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG22	8	0.44
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG23	8	0.44
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	6	0.44
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	6	0.44
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	6	0.44
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD2	3	0.44
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD3	3	0.44
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD2	9	0.44
(1,1965)	1:184:A:LYS:HA	1:184:A:LYS:HD3	9	0.44
(1,1954)	1:140:A:GLU:HG2	1:140:A:GLU:H	6	0.44
(1,1930)	1:158:A:HIS:HB2	1:160:A:THR:H	6	0.44
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	9	0.44
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	1	0.44
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	7	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	3	0.44
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	1	0.44
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	1	0.44
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	1	0.44
(1,1459)	1:79:A:GLN:HB2	1:82:A:GLY:H	10	0.44
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	3	0.44
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	1	0.44
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	1	0.44
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	1	0.44
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	8	0.44
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	8	0.44
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	8	0.44
(1,467)	1:122:A:CYS:HB3	1:134:A:HIS:H	10	0.44
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD11	4	0.44
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD12	4	0.44
(1,323)	2:201:A:Z90:HAP	1:90:A:LEU:HD13	4	0.44
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	5	0.44
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	5	0.44
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	5	0.44
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	8	0.44
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD11	7	0.44
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD12	7	0.44
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD13	7	0.44
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD21	7	0.44
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD22	7	0.44
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD23	7	0.44
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	3	0.44
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	3	0.44
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	3	0.44
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	3	0.44
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	3	0.44
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	3	0.44
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	7	0.44
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	7	0.44
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	7	0.44
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	7	0.44
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	7	0.44
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	7	0.44
(1,3217)	1:3:A:GLY:HA2	1:43:A:TYR:HE1	7	0.43
(1,3217)	1:3:A:GLY:HA2	1:43:A:TYR:HE2	7	0.43
(1,3216)	1:27:A:LYS:HG2	1:27:A:LYS:H	8	0.43
(1,3197)	1:139:A:ARG:HG2	1:140:A:GLU:H	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2961)	1:123:A:THR:HB	1:124:A:ASP:H	6	0.43
(1,2838)	1:132:A:ILE:HG13	1:133:A:LEU:H	1	0.43
(1,2795)	1:16:A:ASN:HD22	1:16:A:ASN:H	6	0.43
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	3	0.43
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	4	0.43
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	4	0.43
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	4	0.43
(1,2466)	1:95:A:ARG:H	1:93:A:ASN:H	8	0.43
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB1	6	0.43
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB2	6	0.43
(1,2187)	1:130:A:GLY:H	1:125:A:ALA:HB3	6	0.43
(1,2159)	1:131:A:LEU:HA	1:126:A:GLU:H	1	0.43
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD21	1	0.43
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD22	1	0.43
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD23	1	0.43
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD21	1	0.43
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD22	1	0.43
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD23	1	0.43
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD21	1	0.43
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD22	1	0.43
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD23	1	0.43
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	3	0.43
(1,1890)	1:120:A:PHE:H	1:120:A:PHE:HD1	3	0.43
(1,1890)	1:120:A:PHE:H	1:120:A:PHE:HD2	3	0.43
(1,1725)	1:128:A:GLY:H	1:130:A:GLY:H	2	0.43
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD21	10	0.43
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD22	10	0.43
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD23	10	0.43
(1,1619)	1:99:A:GLN:HA	1:99:A:GLN:HE22	9	0.43
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	8	0.43
(1,1447)	1:146:A:VAL:HB	1:148:A:GLY:H	9	0.43
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	2	0.43
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	2	0.43
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	2	0.43
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	5	0.43
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	5	0.43
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	5	0.43
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	5	0.43
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	5	0.43
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	5	0.43
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	5	0.43
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	5	0.43
(1,1156)	1:100:A:ASN:HB3	1:99:A:GLN:H	7	0.43
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	6	0.43
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	4	0.43
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	4	0.43
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	4	0.43
(1,853)	1:171:A:ASN:HD22	1:173:A:GLU:H	8	0.43
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	5	0.43
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	5	0.43
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	5	0.43
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	3	0.43
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	3	0.43
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	3	0.43
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	8	0.43
(1,626)	1:177:A:THR:HB	1:170:A:ARG:H	6	0.43
(1,601)	1:170:A:ARG:HG2	1:171:A:ASN:H	8	0.43
(1,566)	1:61:A:LEU:H	1:57:A:LYS:H	1	0.43
(1,338)	1:139:A:ARG:HG2	1:49:A:TYR:HE1	8	0.43
(1,338)	1:139:A:ARG:HG2	1:49:A:TYR:HE2	8	0.43
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	1	0.43
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	1	0.43
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	1	0.43
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	10	0.43
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	10	0.43
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	10	0.43
(1,99)	1:125:A:ALA:HA	1:132:A:ILE:H	3	0.43
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	1	0.43
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	1	0.43
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD11	8	0.42
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD12	8	0.42
(1,3411)	2:201:A:Z90:HAP	1:101:A:LEU:HD13	8	0.42
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	9	0.42
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	9	0.42
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	9	0.42
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	9	0.42
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	9	0.42
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	9	0.42
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	9	0.42
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	9	0.42
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	9	0.42
(1,3358)	1:75:A:PHE:HE1	1:157:A:ILE:H	5	0.42
(1,3358)	1:75:A:PHE:HE2	1:157:A:ILE:H	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3297)	1:143:A:GLN:HE22	1:142:A:LEU:H	1	0.42
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG11	6	0.42
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG12	6	0.42
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG13	6	0.42
(1,2884)	1:131:A:LEU:HB3	1:130:A:GLY:H	4	0.42
(1,2838)	1:132:A:ILE:HG13	1:133:A:LEU:H	4	0.42
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB1	7	0.42
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB2	7	0.42
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB3	7	0.42
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD11	4	0.42
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD12	4	0.42
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD13	4	0.42
(1,2436)	1:66:A:ILE:HG12	1:56:A:SER:H	2	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	1	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	1	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	1	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	2	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	2	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	2	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	3	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	3	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	3	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	4	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	4	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	4	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	5	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	5	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	5	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	6	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	6	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	6	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	7	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	7	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	7	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	8	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	8	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	8	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	9	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	9	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	9	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG21	10	0.42
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG22	10	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2348)	1:111:A:ILE:HB	1:111:A:ILE:HG23	10	0.42
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB2	1	0.42
(1,2275)	1:58:A:VAL:HB	1:57:A:LYS:HB3	1	0.42
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	8	0.42
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	8	0.42
(1,2175)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	8	0.42
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	8	0.42
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	8	0.42
(1,2175)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	8	0.42
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	8	0.42
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	8	0.42
(1,2175)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	8	0.42
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	3	0.42
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	6	0.42
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG21	3	0.42
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG22	3	0.42
(1,2091)	1:168:A:GLN:H	1:166:A:VAL:HG23	3	0.42
(1,1953)	1:175:A:ASP:H	1:170:A:ARG:HG2	4	0.42
(1,1935)	1:135:A:TYR:HD1	1:119:A:SER:H	5	0.42
(1,1935)	1:135:A:TYR:HD2	1:119:A:SER:H	5	0.42
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	3	0.42
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	3	0.42
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	3	0.42
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	10	0.42
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	10	0.42
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	10	0.42
(1,1752)	1:43:A:TYR:HE1	1:37:A:PHE:HE1	1	0.42
(1,1752)	1:43:A:TYR:HE1	1:37:A:PHE:HE2	1	0.42
(1,1752)	1:43:A:TYR:HE2	1:37:A:PHE:HE1	1	0.42
(1,1752)	1:43:A:TYR:HE2	1:37:A:PHE:HE2	1	0.42
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	2	0.42
(1,1725)	1:128:A:GLY:H	1:130:A:GLY:H	8	0.42
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG21	10	0.42
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG22	10	0.42
(1,1641)	1:179:A:PHE:HD1	1:147:A:ILE:HG23	10	0.42
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG21	10	0.42
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG22	10	0.42
(1,1641)	1:179:A:PHE:HD2	1:147:A:ILE:HG23	10	0.42
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	6	0.42
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	6	0.42
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	6	0.42
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	6	0.42
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	6	0.42
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	6	0.42
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	6	0.42
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	6	0.42
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	6	0.42
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	6	0.42
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	6	0.42
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	6	0.42
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	6	0.42
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	6	0.42
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	6	0.42
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	6	0.42
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	6	0.42
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	2	0.42
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD21	9	0.42
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD22	9	0.42
(1,1544)	1:49:A:TYR:HD1	1:142:A:LEU:HD23	9	0.42
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD21	9	0.42
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD22	9	0.42
(1,1544)	1:49:A:TYR:HD2	1:142:A:LEU:HD23	9	0.42
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD11	6	0.42
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD12	6	0.42
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD13	6	0.42
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD11	6	0.42
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD12	6	0.42
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD13	6	0.42
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD11	6	0.42
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD12	6	0.42
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD13	6	0.42
(1,1415)	1:34:A:GLU:HA	1:36:A:GLN:H	9	0.42
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	7	0.42
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	7	0.42
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	7	0.42
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD21	10	0.42
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD22	10	0.42
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD23	10	0.42
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	1	0.42
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	1	0.42
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	1	0.42
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	1	0.42
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	1	0.42
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	1	0.42
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	1	0.42
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	1	0.42
(1,601)	1:170:A:ARG:HG2	1:171:A:ASN:H	7	0.42
(1,454)	1:176:A:HIS:H	1:170:A:ARG:HA	7	0.42
(1,334)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	3	0.42
(1,334)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	3	0.42
(1,334)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	3	0.42
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	3	0.42
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	3	0.42
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	4	0.42
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	4	0.42
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	1	0.42
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	1	0.42
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	1	0.42
(1,231)	1:145:A:ILE:HG21	1:144:A:ASP:H	4	0.42
(1,231)	1:145:A:ILE:HG22	1:144:A:ASP:H	4	0.42
(1,231)	1:145:A:ILE:HG23	1:144:A:ASP:H	4	0.42
(1,167)	1:174:A:CYS:H	1:170:A:ARG:HA	3	0.42
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	3	0.42
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	10	0.42
(1,105)	1:165:A:LYS:H	1:182:A:GLU:H	6	0.42
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	2	0.42
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	2	0.42
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	2	0.42
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	2	0.42
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	2	0.42
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	2	0.42
(1,3583)	1:140:A:GLU:HG2	1:169:A:GLN:HE22	7	0.41
(1,3466)	1:93:A:ASN:HA	1:96:A:GLU:H	4	0.41
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG11	10	0.41
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG12	10	0.41
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG13	10	0.41
(1,3216)	1:27:A:LYS:HG2	1:27:A:LYS:H	10	0.41
(1,3185)	1:16:A:ASN:HD22	1:16:A:ASN:H	3	0.41
(1,3183)	1:175:A:ASP:H	1:174:A:CYS:HB2	1	0.41
(1,2780)	1:26:A:LYS:HG3	1:22:A:TRP:HE1	2	0.41
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD21	10	0.41
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD22	10	0.41
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD23	10	0.41
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2118)	1:94:A:VAL:HG21	1:96:A:GLU:H	6	0.41
(1,2118)	1:94:A:VAL:HG22	1:96:A:GLU:H	6	0.41
(1,2118)	1:94:A:VAL:HG23	1:96:A:GLU:H	6	0.41
(1,2116)	1:161:A:GLU:HG3	1:160:A:THR:HA	3	0.41
(1,2003)	1:48:A:THR:HB	1:47:A:LYS:H	7	0.41
(1,1992)	1:92:A:SER:HB2	1:93:A:ASN:HD22	1	0.41
(1,1852)	1:124:A:ASP:HA	1:130:A:GLY:H	3	0.41
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	1	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	3	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	3	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	3	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	7	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	7	0.41
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	7	0.41
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD21	5	0.41
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD22	5	0.41
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD23	5	0.41
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD11	6	0.41
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD12	6	0.41
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD13	6	0.41
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	9	0.41
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	9	0.41
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	9	0.41
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	7	0.41
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	7	0.41
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	7	0.41
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	7	0.41
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	7	0.41
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	7	0.41
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	7	0.41
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	7	0.41
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	7	0.41
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	9	0.41
(1,965)	1:10:A:GLU:HA	1:51:A:LEU:HD21	7	0.41
(1,965)	1:10:A:GLU:HA	1:51:A:LEU:HD22	7	0.41
(1,965)	1:10:A:GLU:HA	1:51:A:LEU:HD23	7	0.41
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG11	10	0.41
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG12	10	0.41
(1,694)	1:165:A:LYS:HB3	1:166:A:VAL:HG13	10	0.41
(1,522)	1:96:A:GLU:HG2	1:93:A:ASN:H	5	0.41
(1,408)	1:127:A:LYS:HG3	1:126:A:GLU:H	7	0.41
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG21	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG22	2	0.41
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG23	2	0.41
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	2	0.41
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	5	0.41
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	5	0.41
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	5	0.41
(1,261)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	4	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	6	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	6	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	6	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	6	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	6	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	6	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD11	8	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD12	8	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD13	8	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD21	8	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD22	8	0.41
(1,215)	1:32:A:ASP:H	1:31:A:LEU:HD23	8	0.41
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	6	0.41
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	9	0.41
(1,105)	1:182:A:GLU:H	1:164:A:MET:H	9	0.41
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	9	0.41
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD12	9	0.41
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	9	0.41
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD21	9	0.41
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD22	9	0.41
(1,27)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	9	0.41
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG21	5	0.4
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG22	5	0.4
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG23	5	0.4
(1,3216)	1:27:A:LYS:HG2	1:27:A:LYS:H	5	0.4
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	3	0.4
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	3	0.4
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	3	0.4
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	5	0.4
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	5	0.4
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	5	0.4
(1,2993)	1:183:A:GLU:HB2	1:163:A:ASP:H	4	0.4
(1,2795)	1:16:A:ASN:HD22	1:16:A:ASN:H	1	0.4
(1,2660)	1:184:A:LYS:HE3	1:184:A:LYS:H	8	0.4
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG21	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG22	9	0.4
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG23	9	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	1	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	1	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	1	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	1	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	2	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	2	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	2	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	2	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	3	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	3	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	3	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	3	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	5	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	5	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	5	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	5	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	7	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	7	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	7	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	7	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	8	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	8	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	8	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	8	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	9	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	9	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	9	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	9	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	10	0.4
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	10	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	10	0.4
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	10	0.4
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD11	2	0.4
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD12	2	0.4
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD13	2	0.4
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	6	0.4
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	6	0.4
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	6	0.4
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	9	0.4
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	9	0.4
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	7	0.4
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	9	0.4
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD21	10	0.4
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD22	10	0.4
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD23	10	0.4
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD21	10	0.4
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD22	10	0.4
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD23	10	0.4
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD21	10	0.4
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD22	10	0.4
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD23	10	0.4
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	7	0.4
(1,1859)	1:134:A:HIS:HD2	1:122:A:CYS:H	7	0.4
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	5	0.4
(1,1751)	1:161:A:GLU:HG3	1:162:A:ILE:H	2	0.4
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD11	8	0.4
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD12	8	0.4
(1,1430)	1:149:A:ILE:HG21	1:150:A:ILE:HD13	8	0.4
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD11	8	0.4
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD12	8	0.4
(1,1430)	1:149:A:ILE:HG22	1:150:A:ILE:HD13	8	0.4
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD11	8	0.4
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD12	8	0.4
(1,1430)	1:149:A:ILE:HG23	1:150:A:ILE:HD13	8	0.4
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	4	0.4
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD21	10	0.4
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD22	10	0.4
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD23	10	0.4
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD21	10	0.4
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD22	10	0.4
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD23	10	0.4
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD21	10	0.4
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD22	10	0.4
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD23	10	0.4
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	6	0.4
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	9	0.4
(1,798)	1:183:A:GLU:HA	1:162:A:ILE:HA	7	0.4
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	5	0.4
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	5	0.4
(1,614)	1:170:A:ARG:HG2	1:170:A:ARG:H	1	0.4
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	6	0.4
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	6	0.4
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	6	0.4
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	6	0.4
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	6	0.4
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	4	0.4
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	4	0.4
(1,310)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	4	0.4
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	10	0.4
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	3	0.4
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	5	0.4
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	5	0.4
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	10	0.4
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	10	0.4
(1,268)	1:101:A:LEU:HD21	2:201:A:Z90:HAI	8	0.4
(1,268)	1:101:A:LEU:HD22	2:201:A:Z90:HAI	8	0.4
(1,268)	1:101:A:LEU:HD23	2:201:A:Z90:HAI	8	0.4
(1,121)	1:30:A:GLN:HG2	1:31:A:LEU:H	4	0.4
(1,121)	1:30:A:GLN:HG3	1:31:A:LEU:H	4	0.4
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD11	5	0.4
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD12	5	0.4
(1,79)	1:26:A:LYS:HB2	1:51:A:LEU:HD13	5	0.4
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	1	0.39
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	1	0.39
(1,3415)	1:126:A:GLU:HB2	1:127:A:LYS:H	1	0.39
(1,3415)	1:126:A:GLU:HB3	1:127:A:LYS:H	1	0.39
(1,3284)	1:100:A:ASN:HB3	1:103:A:ALA:H	10	0.39
(1,3137)	1:19:A:PRO:HD3	1:22:A:TRP:H	7	0.39
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD11	4	0.39
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD12	4	0.39
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD13	4	0.39
(1,2786)	1:14:A:ILE:HG13	1:22:A:TRP:HE1	5	0.39
(1,2681)	1:181:A:ILE:HB	1:183:A:GLU:H	6	0.39
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD21	9	0.39
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD22	9	0.39
(1,2635)	1:99:A:GLN:HB3	1:98:A:LEU:HD23	9	0.39
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	4	0.39
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	4	0.39
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	4	0.39
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	4	0.39
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG2	6	0.39
(1,2473)	1:40:A:ARG:HB2	1:40:A:ARG:HG3	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG2	6	0.39
(1,2473)	1:40:A:ARG:HB3	1:40:A:ARG:HG3	6	0.39
(1,2273)	1:11:A:LEU:HB3	1:8:A:ALA:H	7	0.39
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	2	0.39
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	2	0.39
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	2	0.39
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG21	2	0.39
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG22	2	0.39
(1,1856)	1:150:A:ILE:H	1:147:A:ILE:HG23	2	0.39
(1,1817)	1:66:A:ILE:HB	1:56:A:SER:H	8	0.39
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	10	0.39
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG21	7	0.39
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG22	7	0.39
(1,1410)	1:94:A:VAL:HG11	1:162:A:ILE:HG23	7	0.39
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG21	7	0.39
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG22	7	0.39
(1,1410)	1:94:A:VAL:HG12	1:162:A:ILE:HG23	7	0.39
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG21	7	0.39
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG22	7	0.39
(1,1410)	1:94:A:VAL:HG13	1:162:A:ILE:HG23	7	0.39
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	7	0.39
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	7	0.39
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	7	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	1	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	1	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	1	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	3	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	3	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	3	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	4	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	4	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	4	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	5	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	5	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	5	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	6	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	6	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	6	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	7	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	7	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	7	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	8	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	8	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	9	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	9	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	9	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	10	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	10	0.39
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	10	0.39
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	10	0.39
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	10	0.39
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	10	0.39
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	3	0.39
(1,798)	1:183:A:GLU:HA	1:162:A:ILE:HA	8	0.39
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	9	0.39
(1,736)	1:108:A:LEU:HA	1:110:A:THR:H	10	0.39
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	2	0.39
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	2	0.39
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	2	0.39
(1,379)	1:95:A:ARG:HD2	1:94:A:VAL:HG11	3	0.39
(1,379)	1:95:A:ARG:HD2	1:94:A:VAL:HG12	3	0.39
(1,379)	1:95:A:ARG:HD2	1:94:A:VAL:HG13	3	0.39
(1,379)	1:95:A:ARG:HD3	1:94:A:VAL:HG11	3	0.39
(1,379)	1:95:A:ARG:HD3	1:94:A:VAL:HG12	3	0.39
(1,379)	1:95:A:ARG:HD3	1:94:A:VAL:HG13	3	0.39
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	9	0.39
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	9	0.39
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG11	10	0.39
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG12	10	0.39
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG13	10	0.39
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG21	10	0.39
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG22	10	0.39
(1,246)	1:28:A:GLU:H	1:58:A:VAL:HG23	10	0.39
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB1	6	0.39
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB2	6	0.39
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB3	6	0.39
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	7	0.39
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	7	0.39
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	7	0.39
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	10	0.39
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	10	0.39
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	10	0.39
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG11	3	0.38
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG12	3	0.38
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG13	3	0.38
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	3	0.38
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	9	0.38
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB1	3	0.38
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB2	3	0.38
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB3	3	0.38
(1,3039)	1:32:A:ASP:HB3	1:27:A:LYS:HA	10	0.38
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD1	9	0.38
(1,2707)	1:7:A:HIS:HD2	1:77:A:PHE:HD2	9	0.38
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	7	0.38
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	7	0.38
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	7	0.38
(1,2005)	1:47:A:LYS:HE3	1:47:A:LYS:H	5	0.38
(1,2005)	1:47:A:LYS:HE3	1:47:A:LYS:H	7	0.38
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	3	0.38
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	8	0.38
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	6	0.38
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	6	0.38
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	6	0.38
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD11	2	0.38
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD12	2	0.38
(1,1329)	1:145:A:ILE:HG12	1:145:A:ILE:HD13	2	0.38
(1,1156)	1:100:A:ASN:HB3	1:99:A:GLN:H	1	0.38
(1,1146)	1:100:A:ASN:HD22	1:99:A:GLN:H	8	0.38
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	2	0.38
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	7	0.38
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	8	0.38
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	10	0.38
(1,874)	1:52:A:VAL:HB	1:67:A:LEU:H	7	0.38
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	6	0.38
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	4	0.38
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	6	0.38
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD21	4	0.38
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD22	4	0.38
(1,746)	1:98:A:LEU:HD21	1:133:A:LEU:HD23	4	0.38
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD21	4	0.38
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD22	4	0.38
(1,746)	1:98:A:LEU:HD22	1:133:A:LEU:HD23	4	0.38
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD21	4	0.38
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD22	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:98:A:LEU:HD23	1:133:A:LEU:HD23	4	0.38
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	7	0.38
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	7	0.38
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	7	0.38
(1,670)	1:143:A:GLN:HG3	1:142:A:LEU:H	10	0.38
(1,614)	1:170:A:ARG:HG2	1:170:A:ARG:H	4	0.38
(1,614)	1:170:A:ARG:HG2	1:170:A:ARG:H	5	0.38
(1,579)	1:173:A:GLU:HB2	1:171:A:ASN:H	5	0.38
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	9	0.38
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	9	0.38
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	9	0.38
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	8	0.38
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	8	0.38
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	8	0.38
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	8	0.38
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	8	0.38
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	8	0.38
(1,266)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	5	0.38
(1,266)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	5	0.38
(1,266)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	5	0.38
(1,231)	1:145:A:ILE:HG21	1:144:A:ASP:H	6	0.38
(1,231)	1:145:A:ILE:HG22	1:144:A:ASP:H	6	0.38
(1,231)	1:145:A:ILE:HG23	1:144:A:ASP:H	6	0.38
(1,213)	1:30:A:GLN:H	1:31:A:LEU:HD11	9	0.38
(1,213)	1:30:A:GLN:H	1:31:A:LEU:HD12	9	0.38
(1,213)	1:30:A:GLN:H	1:31:A:LEU:HD13	9	0.38
(1,213)	1:30:A:GLN:H	1:31:A:LEU:HD21	9	0.38
(1,213)	1:30:A:GLN:H	1:31:A:LEU:HD22	9	0.38
(1,213)	1:30:A:GLN:H	1:31:A:LEU:HD23	9	0.38
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	5	0.38
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	5	0.38
(1,121)	1:30:A:GLN:HG2	1:31:A:LEU:H	5	0.38
(1,121)	1:30:A:GLN:HG3	1:31:A:LEU:H	5	0.38
(2,3)	1:139:A:ARG:HH12	2:201:A:Z90:OAA	2	0.37
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD21	9	0.37
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD22	9	0.37
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD23	9	0.37
(1,3461)	1:132:A:ILE:HG12	1:125:A:ALA:H	6	0.37
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	10	0.37
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD21	10	0.37
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD22	10	0.37
(1,3036)	1:104:A:LEU:HD11	1:101:A:LEU:HD23	10	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD21	10	0.37
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD22	10	0.37
(1,3036)	1:104:A:LEU:HD12	1:101:A:LEU:HD23	10	0.37
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD21	10	0.37
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD22	10	0.37
(1,3036)	1:104:A:LEU:HD13	1:101:A:LEU:HD23	10	0.37
(1,2972)	1:56:A:SER:HB2	1:63:A:ALA:HB1	6	0.37
(1,2972)	1:56:A:SER:HB2	1:63:A:ALA:HB2	6	0.37
(1,2972)	1:56:A:SER:HB2	1:63:A:ALA:HB3	6	0.37
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	5	0.37
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD21	2	0.37
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD22	2	0.37
(1,2854)	1:131:A:LEU:HG	1:133:A:LEU:HD23	2	0.37
(1,2841)	1:65:A:GLU:HG2	1:65:A:GLU:H	9	0.37
(1,2841)	1:65:A:GLU:HG3	1:65:A:GLU:H	9	0.37
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG21	3	0.37
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG22	3	0.37
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG23	3	0.37
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	9	0.37
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	9	0.37
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	9	0.37
(1,2421)	1:72:A:LYS:H	1:148:A:GLY:H	6	0.37
(1,2196)	1:164:A:MET:HA	1:165:A:LYS:HD2	3	0.37
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB1	6	0.37
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB2	6	0.37
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB3	6	0.37
(1,1669)	1:49:A:TYR:HB2	1:53:A:ALA:H	2	0.37
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG21	3	0.37
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG22	3	0.37
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG23	3	0.37
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	8	0.37
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	8	0.37
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	8	0.37
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	5	0.37
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	5	0.37
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	5	0.37
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	5	0.37
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	5	0.37
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	5	0.37
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	5	0.37
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	5	0.37
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD11	2	0.37
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD12	2	0.37
(1,1228)	1:150:A:ILE:HD11	1:147:A:ILE:HD13	2	0.37
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD11	2	0.37
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD12	2	0.37
(1,1228)	1:150:A:ILE:HD12	1:147:A:ILE:HD13	2	0.37
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD11	2	0.37
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD12	2	0.37
(1,1228)	1:150:A:ILE:HD13	1:147:A:ILE:HD13	2	0.37
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	5	0.37
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	9	0.37
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	9	0.37
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	9	0.37
(1,969)	1:153:A:VAL:HB	1:155:A:GLN:H	6	0.37
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	5	0.37
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	7	0.37
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	8	0.37
(1,853)	1:171:A:ASN:HD22	1:173:A:GLU:H	1	0.37
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	2	0.37
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD11	6	0.37
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD12	6	0.37
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD13	6	0.37
(1,501)	1:126:A:GLU:HG3	1:126:A:GLU:H	10	0.37
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE1	7	0.37
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE2	7	0.37
(1,327)	2:201:A:Z90:HAR	1:115:A:MET:HE3	7	0.37
(1,297)	2:201:A:Z90:HAP	2:201:A:Z90:HAM	2	0.37
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG12	4	0.37
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG13	4	0.37
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB1	5	0.37
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB2	5	0.37
(1,220)	1:57:A:LYS:H	1:53:A:ALA:HB3	5	0.37
(1,121)	1:30:A:GLN:HB3	1:31:A:LEU:H	7	0.37
(1,3507)	1:46:A:SER:H	1:47:A:LYS:HE3	1	0.36
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	4	0.36
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	4	0.36
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	4	0.36
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	4	0.36
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	4	0.36
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	4	0.36
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	4	0.36
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	4	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	4	0.36
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD11	9	0.36
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD12	9	0.36
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD13	9	0.36
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	1	0.36
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	8	0.36
(1,3289)	1:63:A:ALA:HB1	1:67:A:LEU:H	9	0.36
(1,3289)	1:63:A:ALA:HB2	1:67:A:LEU:H	9	0.36
(1,3289)	1:63:A:ALA:HB3	1:67:A:LEU:H	9	0.36
(1,3235)	1:32:A:ASP:HB2	1:27:A:LYS:H	6	0.36
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	2	0.36
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	2	0.36
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	2	0.36
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	10	0.36
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	10	0.36
(1,2870)	1:171:A:ASN:HD22	1:171:A:ASN:H	3	0.36
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	3	0.36
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	3	0.36
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	3	0.36
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB1	6	0.36
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB2	6	0.36
(1,2722)	1:53:A:ALA:H	1:29:A:ALA:HB3	6	0.36
(1,2719)	1:149:A:ILE:HA	1:149:A:ILE:HD11	10	0.36
(1,2719)	1:149:A:ILE:HA	1:149:A:ILE:HD12	10	0.36
(1,2719)	1:149:A:ILE:HA	1:149:A:ILE:HD13	10	0.36
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG21	5	0.36
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG22	5	0.36
(1,2705)	1:154:A:ALA:HA	1:153:A:VAL:HG23	5	0.36
(1,2394)	1:17:A:TYR:HE1	1:13:A:VAL:H	3	0.36
(1,2394)	1:17:A:TYR:HE2	1:13:A:VAL:H	3	0.36
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	9	0.36
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	1	0.36
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	2	0.36
(1,2019)	1:83:A:TYR:H	1:83:A:TYR:HD1	5	0.36
(1,2019)	1:83:A:TYR:H	1:83:A:TYR:HD2	5	0.36
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	5	0.36
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	5	0.36
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD21	5	0.36
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD22	5	0.36
(1,1288)	1:150:A:ILE:HG21	1:133:A:LEU:HD23	5	0.36
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD21	5	0.36
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD22	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:150:A:ILE:HG22	1:133:A:LEU:HD23	5	0.36
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD21	5	0.36
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD22	5	0.36
(1,1288)	1:150:A:ILE:HG23	1:133:A:LEU:HD23	5	0.36
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD11	1	0.36
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD12	1	0.36
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD13	1	0.36
(1,1166)	1:159:A:GLY:H	1:157:A:ILE:HG21	6	0.36
(1,1166)	1:159:A:GLY:H	1:157:A:ILE:HG22	6	0.36
(1,1166)	1:159:A:GLY:H	1:157:A:ILE:HG23	6	0.36
(1,1066)	1:139:A:ARG:HG3	1:140:A:GLU:H	9	0.36
(1,984)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	7	0.36
(1,798)	1:183:A:GLU:HA	1:162:A:ILE:HA	4	0.36
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	1	0.36
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	3	0.36
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	5	0.36
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	6	0.36
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	6	0.36
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	6	0.36
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG21	10	0.36
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG22	10	0.36
(1,634)	1:184:A:LYS:H	1:181:A:ILE:HG23	10	0.36
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG21	5	0.36
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG22	5	0.36
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG23	5	0.36
(1,576)	1:171:A:ASN:H	1:169:A:GLN:HA	6	0.36
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	4	0.36
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	10	0.36
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	7	0.36
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	7	0.36
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	7	0.36
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	7	0.36
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	7	0.36
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	7	0.36
(1,311)	1:39:A:VAL:HG11	2:201:A:Z90:HAE	8	0.36
(1,311)	1:39:A:VAL:HG12	2:201:A:Z90:HAE	8	0.36
(1,311)	1:39:A:VAL:HG13	2:201:A:Z90:HAE	8	0.36
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZ	1	0.36
(1,302)	2:201:A:Z90:HAR	2:201:A:Z90:HAZA	1	0.36
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	1	0.36
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	1	0.36
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	7	0.36
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	8	0.36
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	8	0.36
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	8	0.36
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	10	0.36
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	10	0.36
(1,267)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	10	0.36
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	1	0.36
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	1	0.36
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	1	0.36
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	1	0.36
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	1	0.36
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	1	0.36
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	2	0.36
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	2	0.36
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	2	0.36
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	2	0.36
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	2	0.36
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	2	0.36
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	4	0.36
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	4	0.36
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	4	0.35
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	5	0.35
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	6	0.35
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD21	6	0.35
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD22	6	0.35
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD23	6	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	1	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	1	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	1	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	3	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	3	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	3	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	4	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	4	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	4	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	5	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	5	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	5	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	6	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	6	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	7	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	7	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	7	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	8	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	8	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	8	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	9	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	9	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	9	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG21	10	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG22	10	0.35
(1,3120)	1:177:A:THR:HB	1:177:A:THR:HG23	10	0.35
(1,3087)	1:26:A:LYS:HE3	1:22:A:TRP:HE1	9	0.35
(1,2838)	1:132:A:ILE:HG13	1:133:A:LEU:H	8	0.35
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	9	0.35
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	9	0.35
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	9	0.35
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	9	0.35
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	9	0.35
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	9	0.35
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	9	0.35
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	9	0.35
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	9	0.35
(1,2673)	1:34:A:GLU:HA	1:35:A:GLY:H	2	0.35
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	5	0.35
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	5	0.35
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	5	0.35
(1,2436)	1:66:A:ILE:HG12	1:56:A:SER:H	3	0.35
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD21	10	0.35
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD22	10	0.35
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD23	10	0.35
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD21	10	0.35
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD22	10	0.35
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD23	10	0.35
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	8	0.35
(1,2240)	1:155:A:GLN:HA	1:161:A:GLU:H	4	0.35
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG21	4	0.35
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG22	4	0.35
(1,2123)	1:165:A:LYS:HE2	1:167:A:ILE:HG23	4	0.35
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	10	0.35
(1,2042)	1:176:A:HIS:H	1:174:A:CYS:H	9	0.35
(1,1988)	1:26:A:LYS:HB3	1:23:A:GLU:H	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1935)	1:135:A:TYR:HD1	1:119:A:SER:H	2	0.35
(1,1935)	1:135:A:TYR:HD2	1:119:A:SER:H	2	0.35
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	1	0.35
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	1	0.35
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	3	0.35
(1,1504)	1:145:A:ILE:H	1:67:A:LEU:HD21	5	0.35
(1,1504)	1:145:A:ILE:H	1:67:A:LEU:HD22	5	0.35
(1,1504)	1:145:A:ILE:H	1:67:A:LEU:HD23	5	0.35
(1,1472)	1:104:A:LEU:HD21	2:201:A:Z90:HAP	1	0.35
(1,1472)	1:104:A:LEU:HD22	2:201:A:Z90:HAP	1	0.35
(1,1472)	1:104:A:LEU:HD23	2:201:A:Z90:HAP	1	0.35
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	10	0.35
(1,1297)	1:145:A:ILE:HG12	1:71:A:GLY:H	3	0.35
(1,1052)	1:36:A:GLN:H	1:35:A:GLY:H	8	0.35
(1,1038)	1:177:A:THR:HA	1:169:A:GLN:H	7	0.35
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	4	0.35
(1,874)	1:52:A:VAL:HB	1:67:A:LEU:H	8	0.35
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	4	0.35
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	7	0.35
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	10	0.35
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	1	0.35
(1,596)	1:170:A:ARG:HG3	1:170:A:ARG:H	5	0.35
(1,576)	1:171:A:ASN:H	1:169:A:GLN:HA	9	0.35
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	4	0.35
(1,467)	1:122:A:CYS:HB3	1:134:A:HIS:H	3	0.35
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG21	4	0.35
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG22	4	0.35
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG23	4	0.35
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD11	8	0.35
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD12	8	0.35
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD13	8	0.35
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD21	8	0.35
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD22	8	0.35
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD23	8	0.35
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	10	0.35
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	10	0.35
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	10	0.35
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	10	0.35
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	10	0.35
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	10	0.35
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	8	0.35
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	8	0.35
(1,311)	1:39:A:VAL:HG11	2:201:A:Z90:HAE	5	0.35
(1,311)	1:39:A:VAL:HG12	2:201:A:Z90:HAE	5	0.35
(1,311)	1:39:A:VAL:HG13	2:201:A:Z90:HAE	5	0.35
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	2	0.35
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	2	0.35
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	8	0.35
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	8	0.35
(1,262)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	3	0.35
(1,262)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	10	0.35
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	5	0.35
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	5	0.35
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	5	0.35
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG12	7	0.35
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG13	7	0.35
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	7	0.35
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	7	0.35
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	7	0.35
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	7	0.35
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	7	0.35
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	7	0.35
(1,188)	1:165:A:LYS:HD2	1:166:A:VAL:H	8	0.35
(1,188)	1:165:A:LYS:HD3	1:166:A:VAL:H	8	0.35
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	2	0.35
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	2	0.35
(1,137)	1:56:A:SER:HB2	1:62:A:ASN:H	4	0.35
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	7	0.35
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	7	0.35
(1,3484)	1:37:A:PHE:H	1:35:A:GLY:H	10	0.34
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	10	0.34
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	10	0.34
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	10	0.34
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	7	0.34
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG11	7	0.34
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG12	7	0.34
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG13	7	0.34
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG21	7	0.34
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG22	7	0.34
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG23	7	0.34
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG11	10	0.34
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG12	10	0.34
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG13	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3233)	1:141:A:GLY:HA2	1:140:A:GLU:H	9	0.34
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	4	0.34
(1,3197)	1:139:A:ARG:HG2	1:140:A:GLU:H	3	0.34
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	2	0.34
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	6	0.34
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	6	0.34
(1,2819)	1:160:A:THR:HB	1:159:A:GLY:H	6	0.34
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	7	0.34
(1,2673)	1:34:A:GLU:HA	1:35:A:GLY:H	4	0.34
(1,2660)	1:184:A:LYS:HE3	1:184:A:LYS:H	6	0.34
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD1	1	0.34
(1,2595)	1:165:A:LYS:HG3	1:179:A:PHE:HD2	1	0.34
(1,2159)	1:131:A:LEU:HA	1:126:A:GLU:H	8	0.34
(1,2130)	1:167:A:ILE:HG12	1:179:A:PHE:H	8	0.34
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG21	5	0.34
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG22	5	0.34
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG23	5	0.34
(1,2042)	1:176:A:HIS:H	1:174:A:CYS:H	7	0.34
(1,1985)	1:136:A:TYR:HD1	1:135:A:TYR:H	9	0.34
(1,1985)	1:136:A:TYR:HD2	1:135:A:TYR:H	9	0.34
(1,1956)	1:34:A:GLU:HB2	1:36:A:GLN:H	1	0.34
(1,1956)	1:34:A:GLU:HB3	1:36:A:GLN:H	1	0.34
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	8	0.34
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	6	0.34
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	6	0.34
(1,1755)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	6	0.34
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG21	9	0.34
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG22	9	0.34
(1,1680)	1:159:A:GLY:H	1:94:A:VAL:HG23	9	0.34
(1,1672)	1:173:A:GLU:HG3	1:174:A:CYS:H	2	0.34
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG21	10	0.34
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG22	10	0.34
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG23	10	0.34
(1,1533)	1:161:A:GLU:HA	1:184:A:LYS:H	10	0.34
(1,1502)	1:57:A:LYS:HG2	1:58:A:VAL:H	8	0.34
(1,1495)	1:125:A:ALA:HB1	1:131:A:LEU:H	5	0.34
(1,1495)	1:125:A:ALA:HB2	1:131:A:LEU:H	5	0.34
(1,1495)	1:125:A:ALA:HB3	1:131:A:LEU:H	5	0.34
(1,1480)	1:171:A:ASN:HD22	1:171:A:ASN:HA	10	0.34
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD11	2	0.34
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD12	2	0.34
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD13	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	5	0.34
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	5	0.34
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	5	0.34
(1,971)	1:92:A:SER:HB3	1:93:A:ASN:H	5	0.34
(1,896)	1:145:A:ILE:HB	1:71:A:GLY:H	7	0.34
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	1	0.34
(1,782)	1:180:A:LEU:HA	1:181:A:ILE:H	8	0.34
(1,781)	1:146:A:VAL:HB	1:150:A:ILE:HD11	5	0.34
(1,781)	1:146:A:VAL:HB	1:150:A:ILE:HD12	5	0.34
(1,781)	1:146:A:VAL:HB	1:150:A:ILE:HD13	5	0.34
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	1	0.34
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	1	0.34
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD11	9	0.34
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD12	9	0.34
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD13	9	0.34
(1,658)	1:142:A:LEU:H	1:141:A:GLY:H	6	0.34
(1,624)	1:92:A:SER:H	1:96:A:GLU:HG3	7	0.34
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE1	4	0.34
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE2	4	0.34
(1,547)	1:11:A:LEU:H	1:73:A:MET:HE3	4	0.34
(1,401)	1:132:A:ILE:HA	1:125:A:ALA:H	10	0.34
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZ	6	0.34
(1,292)	2:201:A:Z90:HAF	2:201:A:Z90:HAZA	6	0.34
(1,270)	1:150:A:ILE:HG21	2:201:A:Z90:HAI	8	0.34
(1,270)	1:150:A:ILE:HG22	2:201:A:Z90:HAI	8	0.34
(1,270)	1:150:A:ILE:HG23	2:201:A:Z90:HAI	8	0.34
(1,262)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	2	0.34
(1,254)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	2	0.34
(1,254)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	2	0.34
(1,254)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	2	0.34
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	1	0.34
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	1	0.34
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	1	0.34
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	1	0.34
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	1	0.34
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	1	0.34
(1,120)	1:27:A:LYS:HD2	1:30:A:GLN:H	7	0.34
(1,120)	1:27:A:LYS:HD3	1:30:A:GLN:H	7	0.34
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	3	0.34
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	3	0.34
(1,49)	1:69:A:MET:HE1	1:61:A:LEU:HD21	1	0.34
(1,49)	1:69:A:MET:HE1	1:61:A:LEU:HD22	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:69:A:MET:HE1	1:61:A:LEU:HD23	1	0.34
(1,49)	1:69:A:MET:HE2	1:61:A:LEU:HD21	1	0.34
(1,49)	1:69:A:MET:HE2	1:61:A:LEU:HD22	1	0.34
(1,49)	1:69:A:MET:HE2	1:61:A:LEU:HD23	1	0.34
(1,49)	1:69:A:MET:HE3	1:61:A:LEU:HD21	1	0.34
(1,49)	1:69:A:MET:HE3	1:61:A:LEU:HD22	1	0.34
(1,49)	1:69:A:MET:HE3	1:61:A:LEU:HD23	1	0.34
(2,2)	2:201:A:Z90:OAC	1:137:A:SER:HG	10	0.33
(1,3565)	1:131:A:LEU:HG	1:181:A:ILE:H	10	0.33
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD11	4	0.33
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD12	4	0.33
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD13	4	0.33
(1,3308)	1:27:A:LYS:HG3	1:28:A:GLU:H	3	0.33
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB1	4	0.33
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB2	4	0.33
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB3	4	0.33
(1,3033)	1:143:A:GLN:HB2	1:166:A:VAL:HG21	7	0.33
(1,3033)	1:143:A:GLN:HB2	1:166:A:VAL:HG22	7	0.33
(1,3033)	1:143:A:GLN:HB2	1:166:A:VAL:HG23	7	0.33
(1,3033)	1:143:A:GLN:HB3	1:166:A:VAL:HG21	7	0.33
(1,3033)	1:143:A:GLN:HB3	1:166:A:VAL:HG22	7	0.33
(1,3033)	1:143:A:GLN:HB3	1:166:A:VAL:HG23	7	0.33
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	4	0.33
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	10	0.33
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	10	0.33
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	10	0.33
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	10	0.33
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	10	0.33
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	10	0.33
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	10	0.33
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	10	0.33
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	10	0.33
(1,2734)	1:14:A:ILE:HB	1:16:A:ASN:H	1	0.33
(1,2681)	1:181:A:ILE:HB	1:183:A:GLU:H	8	0.33
(1,2673)	1:34:A:GLU:HA	1:35:A:GLY:H	6	0.33
(1,2672)	1:179:A:PHE:HE1	1:146:A:VAL:H	8	0.33
(1,2672)	1:179:A:PHE:HE2	1:146:A:VAL:H	8	0.33
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	1	0.33
(1,2509)	1:73:A:MET:H	1:73:A:MET:HE1	4	0.33
(1,2509)	1:73:A:MET:H	1:73:A:MET:HE2	4	0.33
(1,2509)	1:73:A:MET:H	1:73:A:MET:HE3	4	0.33
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD21	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD22	3	0.33
(1,2474)	1:99:A:GLN:HB2	1:98:A:LEU:HD23	3	0.33
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	2	0.33
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	2	0.33
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	2	0.33
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG21	6	0.33
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG22	6	0.33
(1,2317)	1:142:A:LEU:HD21	1:48:A:THR:HG23	6	0.33
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG21	6	0.33
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG22	6	0.33
(1,2317)	1:142:A:LEU:HD22	1:48:A:THR:HG23	6	0.33
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG21	6	0.33
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG22	6	0.33
(1,2317)	1:142:A:LEU:HD23	1:48:A:THR:HG23	6	0.33
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	1	0.33
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	7	0.33
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	1	0.33
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD11	2	0.33
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD12	2	0.33
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD13	2	0.33
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	6	0.33
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	3	0.33
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	9	0.33
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	2	0.33
(1,1810)	1:93:A:ASN:HD22	1:96:A:GLU:HB3	5	0.33
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	8	0.33
(1,1764)	1:49:A:TYR:HB3	1:48:A:THR:H	4	0.33
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD11	3	0.33
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD12	3	0.33
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD13	3	0.33
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD21	3	0.33
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD22	3	0.33
(1,1673)	1:130:A:GLY:H	1:131:A:LEU:HD23	3	0.33
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD11	6	0.33
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD12	6	0.33
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD13	6	0.33
(1,1552)	1:186:A:SER:HB3	1:184:A:LYS:HA	7	0.33
(1,1219)	1:34:A:GLU:H	1:33:A:GLU:HB2	7	0.33
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD11	9	0.33
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD12	9	0.33
(1,1211)	1:64:A:GLY:H	1:67:A:LEU:HD13	9	0.33
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	2	0.33
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	2	0.33
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	9	0.33
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	6	0.33
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	7	0.33
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	7	0.33
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	9	0.33
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	9	0.33
(1,729)	1:142:A:LEU:H	1:141:A:GLY:H	6	0.33
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD11	8	0.33
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD12	8	0.33
(1,716)	1:155:A:GLN:H	1:157:A:ILE:HD13	8	0.33
(1,707)	1:125:A:ALA:HA	1:132:A:ILE:HD11	10	0.33
(1,707)	1:125:A:ALA:HA	1:132:A:ILE:HD12	10	0.33
(1,707)	1:125:A:ALA:HA	1:132:A:ILE:HD13	10	0.33
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	2	0.33
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	2	0.33
(1,650)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	2	0.33
(1,596)	1:170:A:ARG:HG3	1:170:A:ARG:H	1	0.33
(1,564)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	2	0.33
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD11	7	0.33
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD12	7	0.33
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD13	7	0.33
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD21	7	0.33
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD22	7	0.33
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD23	7	0.33
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG11	2	0.33
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG12	2	0.33
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG13	2	0.33
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG21	2	0.33
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG22	2	0.33
(1,325)	2:201:A:Z90:HAH	1:146:A:VAL:HG23	2	0.33
(1,262)	2:201:A:Z90:HAP	2:201:A:Z90:HBDA	6	0.33
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG11	4	0.33
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG12	4	0.33
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG13	4	0.33
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG21	4	0.33
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG22	4	0.33
(1,201)	1:24:A:ASP:H	1:58:A:VAL:HG23	4	0.33
(1,148)	1:145:A:ILE:HG12	1:143:A:GLN:H	1	0.33
(1,148)	1:145:A:ILE:HG13	1:143:A:GLN:H	1	0.33
(1,124)	1:27:A:LYS:HB2	1:32:A:ASP:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:27:A:LYS:HB3	1:32:A:ASP:H	4	0.33
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB1	4	0.33
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB2	4	0.33
(1,68)	1:180:A:LEU:HD11	1:125:A:ALA:HB3	4	0.33
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB1	4	0.33
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB2	4	0.33
(1,68)	1:180:A:LEU:HD12	1:125:A:ALA:HB3	4	0.33
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB1	4	0.33
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB2	4	0.33
(1,68)	1:180:A:LEU:HD13	1:125:A:ALA:HB3	4	0.33
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	10	0.32
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	10	0.32
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	10	0.32
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	4	0.32
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	4	0.32
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	7	0.32
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	7	0.32
(1,3289)	1:63:A:ALA:HB1	1:67:A:LEU:H	6	0.32
(1,3289)	1:63:A:ALA:HB2	1:67:A:LEU:H	6	0.32
(1,3289)	1:63:A:ALA:HB3	1:67:A:LEU:H	6	0.32
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	4	0.32
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	4	0.32
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	4	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD21	1	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD22	1	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD23	1	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD21	8	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD22	8	0.32
(1,2956)	1:62:A:ASN:H	1:61:A:LEU:HD23	8	0.32
(1,2786)	1:14:A:ILE:HG13	1:22:A:TRP:HE1	4	0.32
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	6	0.32
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	6	0.32
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	6	0.32
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	6	0.32
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	6	0.32
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	6	0.32
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	6	0.32
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	6	0.32
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	6	0.32
(1,2725)	1:1:A:MET:HE1	1:48:A:THR:HA	10	0.32
(1,2725)	1:1:A:MET:HE2	1:48:A:THR:HA	10	0.32
(1,2725)	1:1:A:MET:HE3	1:48:A:THR:HA	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	1	0.32
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	1	0.32
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	1	0.32
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	1	0.32
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	1	0.32
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	1	0.32
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	1	0.32
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	1	0.32
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	1	0.32
(1,2680)	1:180:A:LEU:HA	1:167:A:ILE:H	2	0.32
(1,2673)	1:34:A:GLU:HA	1:35:A:GLY:H	10	0.32
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG21	5	0.32
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG22	5	0.32
(1,2455)	1:4:A:PHE:HA	1:39:A:VAL:HG23	5	0.32
(1,2412)	1:24:A:ASP:HB3	1:23:A:GLU:H	5	0.32
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	8	0.32
(1,2273)	1:11:A:LEU:HB3	1:8:A:ALA:H	10	0.32
(1,2188)	1:183:A:GLU:HB2	1:185:A:GLU:H	4	0.32
(1,2141)	1:169:A:GLN:HE22	1:169:A:GLN:H	6	0.32
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	7	0.32
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	10	0.32
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	4	0.32
(1,2027)	2:201:A:Z90:HAE	1:39:A:VAL:HG11	9	0.32
(1,2027)	2:201:A:Z90:HAE	1:39:A:VAL:HG12	9	0.32
(1,2027)	2:201:A:Z90:HAE	1:39:A:VAL:HG13	9	0.32
(1,1960)	1:184:A:LYS:HE2	1:184:A:LYS:HA	1	0.32
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD11	3	0.32
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD12	3	0.32
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD13	3	0.32
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	1	0.32
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD11	4	0.32
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD12	4	0.32
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD13	4	0.32
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD11	4	0.32
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD12	4	0.32
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD13	4	0.32
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD11	4	0.32
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD12	4	0.32
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD13	4	0.32
(1,1733)	1:49:A:TYR:HD1	1:142:A:LEU:H	10	0.32
(1,1733)	1:49:A:TYR:HD2	1:142:A:LEU:H	10	0.32
(1,1715)	1:50:A:ASP:HB2	1:48:A:THR:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD21	6	0.32
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD22	6	0.32
(1,1660)	2:201:A:Z90:HAH	1:104:A:LEU:HD23	6	0.32
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	2	0.32
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB1	9	0.32
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB2	9	0.32
(1,1626)	1:130:A:GLY:H	1:125:A:ALA:HB3	9	0.32
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	2	0.32
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG21	4	0.32
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG22	4	0.32
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG23	4	0.32
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	1	0.32
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	1	0.32
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	1	0.32
(1,1459)	1:79:A:GLN:HB2	1:82:A:GLY:H	2	0.32
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	7	0.32
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	7	0.32
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	6	0.32
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	6	0.32
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	6	0.32
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD11	7	0.32
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD12	7	0.32
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD13	7	0.32
(1,1231)	1:98:A:LEU:HD11	1:134:A:HIS:H	10	0.32
(1,1231)	1:98:A:LEU:HD12	1:134:A:HIS:H	10	0.32
(1,1231)	1:98:A:LEU:HD13	1:134:A:HIS:H	10	0.32
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD11	3	0.32
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD12	3	0.32
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD13	3	0.32
(1,1152)	1:62:A:ASN:HD22	1:63:A:ALA:H	10	0.32
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	1	0.32
(1,948)	1:50:A:ASP:HB2	1:53:A:ALA:H	3	0.32
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	8	0.32
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	8	0.32
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	8	0.32
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	8	0.32
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD21	5	0.32
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD22	5	0.32
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD23	5	0.32
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	4	0.32
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	4	0.32
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	3	0.32
(1,596)	1:170:A:ARG:HG3	1:170:A:ARG:H	4	0.32
(1,467)	1:122:A:CYS:HB3	1:134:A:HIS:H	8	0.32
(1,462)	1:165:A:LYS:HD3	1:180:A:LEU:H	8	0.32
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	8	0.32
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG21	10	0.32
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG22	10	0.32
(1,359)	1:6:A:ASN:HA	1:5:A:VAL:HG23	10	0.32
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG21	9	0.32
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG22	9	0.32
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG23	9	0.32
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	5	0.32
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	5	0.32
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	5	0.32
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	4	0.32
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	8	0.32
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	8	0.32
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	8	0.32
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG11	6	0.32
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG12	6	0.32
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG13	6	0.32
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG21	6	0.32
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG22	6	0.32
(1,205)	1:26:A:LYS:H	1:58:A:VAL:HG23	6	0.32
(1,120)	1:27:A:LYS:HD2	1:30:A:GLN:H	9	0.32
(1,120)	1:27:A:LYS:HD3	1:30:A:GLN:H	9	0.32
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE1	2	0.32
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE2	2	0.32
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE3	2	0.32
(1,3443)	1:143:A:GLN:HG3	1:144:A:ASP:H	3	0.31
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD21	2	0.31
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD22	2	0.31
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD23	2	0.31
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD11	8	0.31
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD12	8	0.31
(1,3375)	1:31:A:LEU:H	1:51:A:LEU:HD13	8	0.31
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	1	0.31
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	1	0.31
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	1	0.31
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	8	0.31
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	8	0.31
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3330)	1:178:A:GLN:HA	1:179:A:PHE:H	2	0.31
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD11	7	0.31
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD12	7	0.31
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD13	7	0.31
(1,3289)	1:63:A:ALA:HB1	1:67:A:LEU:H	5	0.31
(1,3289)	1:63:A:ALA:HB2	1:67:A:LEU:H	5	0.31
(1,3289)	1:63:A:ALA:HB3	1:67:A:LEU:H	5	0.31
(1,3250)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	4	0.31
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG21	1	0.31
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG22	1	0.31
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG23	1	0.31
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	10	0.31
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	10	0.31
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	10	0.31
(1,3149)	1:93:A:ASN:HA	1:95:A:ARG:H	2	0.31
(1,3072)	1:165:A:LYS:HE2	1:165:A:LYS:H	10	0.31
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG21	1	0.31
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG22	1	0.31
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG23	1	0.31
(1,2961)	1:123:A:THR:HB	1:124:A:ASP:H	4	0.31
(1,2930)	1:61:A:LEU:HD11	1:66:A:ILE:H	10	0.31
(1,2930)	1:61:A:LEU:HD12	1:66:A:ILE:H	10	0.31
(1,2930)	1:61:A:LEU:HD13	1:66:A:ILE:H	10	0.31
(1,2884)	1:131:A:LEU:HB3	1:130:A:GLY:H	5	0.31
(1,2863)	1:126:A:GLU:H	1:130:A:GLY:H	3	0.31
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	4	0.31
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	4	0.31
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	4	0.31
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	4	0.31
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	4	0.31
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	4	0.31
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG11	8	0.31
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG12	8	0.31
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG13	8	0.31
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG11	8	0.31
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG12	8	0.31
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG13	8	0.31
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG11	8	0.31
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG12	8	0.31
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG13	8	0.31
(1,2701)	1:99:A:GLN:HE22	1:95:A:ARG:HG3	2	0.31
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB1	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB2	5	0.31
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB3	5	0.31
(1,2565)	1:135:A:TYR:HB2	1:179:A:PHE:H	6	0.31
(1,2513)	1:142:A:LEU:HD21	1:139:A:ARG:H	9	0.31
(1,2513)	1:142:A:LEU:HD22	1:139:A:ARG:H	9	0.31
(1,2513)	1:142:A:LEU:HD23	1:139:A:ARG:H	9	0.31
(1,2466)	1:95:A:ARG:H	1:93:A:ASN:H	6	0.31
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB1	8	0.31
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB2	8	0.31
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB3	8	0.31
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	7	0.31
(1,2273)	1:11:A:LEU:HB3	1:8:A:ALA:H	4	0.31
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	4	0.31
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	6	0.31
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	3	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD11	2	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD12	2	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD13	2	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD11	2	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD12	2	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD13	2	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD11	2	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD12	2	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD13	2	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD11	10	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD12	10	0.31
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD13	10	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD11	10	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD12	10	0.31
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD13	10	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD11	10	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD12	10	0.31
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD13	10	0.31
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	8	0.31
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	8	0.31
(1,1429)	1:72:A:LYS:HA	1:148:A:GLY:H	5	0.31
(1,1345)	1:19:A:PRO:HD2	1:18:A:GLY:H	9	0.31
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG21	1	0.31
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG22	1	0.31
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG23	1	0.31
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD11	9	0.31
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD12	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD13	9	0.31
(1,1274)	1:5:A:VAL:HG11	1:5:A:VAL:H	4	0.31
(1,1274)	1:5:A:VAL:HG12	1:5:A:VAL:H	4	0.31
(1,1274)	1:5:A:VAL:HG13	1:5:A:VAL:H	4	0.31
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	9	0.31
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	9	0.31
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	9	0.31
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	9	0.31
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	9	0.31
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	9	0.31
(1,971)	1:92:A:SER:HB3	1:93:A:ASN:H	4	0.31
(1,971)	1:92:A:SER:HB3	1:93:A:ASN:H	10	0.31
(1,874)	1:52:A:VAL:HB	1:67:A:LEU:H	1	0.31
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	9	0.31
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	10	0.31
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	3	0.31
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	10	0.31
(1,823)	1:183:A:GLU:HA	1:162:A:ILE:H	9	0.31
(1,818)	1:114:A:GLY:H	1:115:A:MET:H	6	0.31
(1,624)	1:92:A:SER:H	1:96:A:GLU:HG3	5	0.31
(1,592)	1:158:A:HIS:HA	1:160:A:THR:H	5	0.31
(1,549)	1:72:A:LYS:H	1:145:A:ILE:HA	5	0.31
(1,525)	1:131:A:LEU:HB2	1:183:A:GLU:H	1	0.31
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG12	9	0.31
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG13	9	0.31
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	8	0.31
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	8	0.31
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	8	0.31
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	8	0.31
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	8	0.31
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	8	0.31
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	7	0.31
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	7	0.31
(1,135)	1:59:A:LEU:HA	1:61:A:LEU:H	2	0.31
(1,114)	1:165:A:LYS:H	1:182:A:GLU:H	6	0.31
(1,97)	1:132:A:ILE:HA	1:131:A:LEU:H	5	0.31
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE1	9	0.31
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE2	9	0.31
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE3	9	0.31
(1,3549)	1:165:A:LYS:HG2	1:180:A:LEU:H	7	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD11	7	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD12	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD13	7	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD21	7	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD22	7	0.3
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD23	7	0.3
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	6	0.3
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	6	0.3
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD11	1	0.3
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD12	1	0.3
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD13	1	0.3
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD11	1	0.3
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD12	1	0.3
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD13	1	0.3
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD11	1	0.3
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD12	1	0.3
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD13	1	0.3
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	10	0.3
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	10	0.3
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	10	0.3
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	10	0.3
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	10	0.3
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	10	0.3
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	10	0.3
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	10	0.3
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	10	0.3
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	4	0.3
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	4	0.3
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	4	0.3
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	7	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	1	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	1	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	1	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	2	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	2	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	2	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	3	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	3	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	3	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	4	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	4	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	4	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	5	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	5	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	6	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	6	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	6	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	7	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	7	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	7	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	8	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	8	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	8	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG21	9	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG22	9	0.3
(1,3157)	1:149:A:ILE:HB	1:149:A:ILE:HG23	9	0.3
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	1	0.3
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	1	0.3
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	1	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	1	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	1	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	1	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	1	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	1	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	1	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	2	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	2	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	2	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	2	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	2	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	2	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	3	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	3	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	3	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	3	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	3	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	3	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	4	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	4	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	4	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	4	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	4	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	4	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	5	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	5	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	5	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	5	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	5	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	6	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	6	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	6	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	6	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	6	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	6	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	7	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	7	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	7	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	7	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	7	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	7	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	8	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	8	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	8	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	8	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	8	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	8	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	9	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	9	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	9	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	9	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	9	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	9	0.3
(1,3022)	1:146:A:VAL:HG11	1:146:A:VAL:HB	10	0.3
(1,3022)	1:146:A:VAL:HG12	1:146:A:VAL:HB	10	0.3
(1,3022)	1:146:A:VAL:HG13	1:146:A:VAL:HB	10	0.3
(1,3022)	1:146:A:VAL:HG21	1:146:A:VAL:HB	10	0.3
(1,3022)	1:146:A:VAL:HG22	1:146:A:VAL:HB	10	0.3
(1,3022)	1:146:A:VAL:HG23	1:146:A:VAL:HB	10	0.3
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	8	0.3
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	8	0.3
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	8	0.3
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	8	0.3
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	8	0.3
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	8	0.3
(1,2771)	1:137:A:SER:HA	1:119:A:SER:H	8	0.3
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	4	0.3
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	4	0.3
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	4	0.3
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	4	0.3
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	4	0.3
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	4	0.3
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	4	0.3
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	4	0.3
(1,2423)	1:183:A:GLU:HB3	1:184:A:LYS:H	3	0.3
(1,2412)	1:24:A:ASP:HB3	1:23:A:GLU:H	10	0.3
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	10	0.3
(1,2196)	1:164:A:MET:HA	1:165:A:LYS:HD2	7	0.3
(1,1988)	1:26:A:LYS:HB3	1:23:A:GLU:H	9	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	2	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	2	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	2	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	2	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	2	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	2	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	3	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	3	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	3	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	3	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	3	0.3
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	3	0.3
(1,1968)	1:3:A:GLY:H	1:43:A:TYR:HE1	1	0.3
(1,1968)	1:3:A:GLY:H	1:43:A:TYR:HE2	1	0.3
(1,1968)	1:3:A:GLY:H	1:43:A:TYR:HE1	5	0.3
(1,1968)	1:3:A:GLY:H	1:43:A:TYR:HE2	5	0.3
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	10	0.3
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD11	7	0.3
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD12	7	0.3
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD13	7	0.3
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	2	0.3
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	4	0.3
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD11	7	0.3
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD12	7	0.3
(1,1559)	1:41:A:ILE:H	1:38:A:LEU:HD13	7	0.3
(1,1480)	1:171:A:ASN:HD22	1:171:A:ASN:HA	2	0.3
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	7	0.3
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	7	0.3
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	7	0.3
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	7	0.3
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	7	0.3
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	7	0.3
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	7	0.3
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	7	0.3
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD21	10	0.3
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD22	10	0.3
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD23	10	0.3
(1,1152)	1:62:A:ASN:HD22	1:63:A:ALA:H	5	0.3
(1,1138)	1:73:A:MET:HE1	1:16:A:ASN:H	6	0.3
(1,1138)	1:73:A:MET:HE2	1:16:A:ASN:H	6	0.3
(1,1138)	1:73:A:MET:HE3	1:16:A:ASN:H	6	0.3
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	1	0.3
(1,1102)	1:160:A:THR:HB	1:159:A:GLY:H	5	0.3
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	8	0.3
(1,1061)	1:54:A:ALA:HA	1:29:A:ALA:H	5	0.3
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	5	0.3
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	6	0.3
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	2	0.3
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	2	0.3
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	2	0.3
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD11	7	0.3
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD12	7	0.3
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD13	7	0.3
(1,800)	1:52:A:VAL:HB	1:66:A:ILE:HG12	5	0.3
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD11	3	0.3
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD12	3	0.3
(1,741)	1:133:A:LEU:H	1:132:A:ILE:HD13	3	0.3
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	8	0.3
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	8	0.3
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	8	0.3
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD11	8	0.3
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD12	8	0.3
(1,701)	1:51:A:LEU:HD11	1:9:A:LEU:HD13	8	0.3
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD11	8	0.3
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD12	8	0.3
(1,701)	1:51:A:LEU:HD12	1:9:A:LEU:HD13	8	0.3
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD11	8	0.3
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD12	8	0.3
(1,701)	1:51:A:LEU:HD13	1:9:A:LEU:HD13	8	0.3
(1,601)	1:170:A:ARG:HG2	1:171:A:ASN:H	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,576)	1:171:A:ASN:H	1:169:A:GLN:HA	3	0.3
(1,529)	1:179:A:PHE:HD1	1:147:A:ILE:H	1	0.3
(1,529)	1:179:A:PHE:HD2	1:147:A:ILE:H	1	0.3
(1,401)	1:132:A:ILE:HA	1:125:A:ALA:H	6	0.3
(1,260)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	1	0.3
(1,260)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	4	0.3
(1,260)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	5	0.3
(1,260)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	9	0.3
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	10	0.3
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	10	0.3
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	10	0.3
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	10	0.3
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	10	0.3
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	10	0.3
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG12	8	0.3
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG13	8	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	2	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	2	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	2	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	2	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	2	0.3
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	2	0.3
(1,183)	1:3:A:GLY:H	1:43:A:TYR:HE1	4	0.3
(1,183)	1:3:A:GLY:H	1:43:A:TYR:HE2	4	0.3
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	3	0.3
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	3	0.3
(1,137)	1:65:A:GLU:HA	1:62:A:ASN:H	7	0.3
(1,114)	1:182:A:GLU:H	1:164:A:MET:H	9	0.3
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB1	5	0.3
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB2	5	0.3
(1,68)	1:131:A:LEU:HD11	1:125:A:ALA:HB3	5	0.3
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB1	5	0.3
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB2	5	0.3
(1,68)	1:131:A:LEU:HD12	1:125:A:ALA:HB3	5	0.3
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB1	5	0.3
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB2	5	0.3
(1,68)	1:131:A:LEU:HD13	1:125:A:ALA:HB3	5	0.3
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB1	5	0.3
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB2	5	0.3
(1,68)	1:131:A:LEU:HD21	1:125:A:ALA:HB3	5	0.3
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB1	5	0.3
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB2	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:131:A:LEU:HD22	1:125:A:ALA:HB3	5	0.3
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB1	5	0.3
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB2	5	0.3
(1,68)	1:131:A:LEU:HD23	1:125:A:ALA:HB3	5	0.3
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE1	7	0.3
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE2	7	0.3
(1,50)	1:69:A:MET:HA	1:69:A:MET:HE3	7	0.3
(2,4)	1:139:A:ARG:HH21	2:201:A:Z90:OAB	9	0.29
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD11	3	0.29
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD12	3	0.29
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD13	3	0.29
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD21	3	0.29
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD22	3	0.29
(1,3486)	1:124:A:ASP:H	1:131:A:LEU:HD23	3	0.29
(1,3197)	1:139:A:ARG:HG2	1:140:A:GLU:H	7	0.29
(1,3183)	1:175:A:ASP:H	1:174:A:CYS:HB2	4	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	2	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	2	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	2	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	3	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	3	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	3	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	4	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	4	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	4	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	5	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	5	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	5	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	6	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	6	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	6	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	7	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	7	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	7	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	8	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	8	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	8	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	9	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	9	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	9	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG21	10	0.29
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG22	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3150)	1:150:A:ILE:HB	1:150:A:ILE:HG23	10	0.29
(1,3068)	1:179:A:PHE:HD1	1:146:A:VAL:H	7	0.29
(1,3068)	1:179:A:PHE:HD2	1:146:A:VAL:H	7	0.29
(1,3043)	1:57:A:LYS:H	1:25:A:ILE:HG12	8	0.29
(1,3043)	1:57:A:LYS:H	1:25:A:ILE:HG13	8	0.29
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG21	1	0.29
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG22	1	0.29
(1,2844)	1:38:A:LEU:HB2	1:39:A:VAL:HG23	1	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	6	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	6	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	6	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	6	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	6	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	6	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	9	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	9	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	9	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	9	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	9	0.29
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	9	0.29
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	3	0.29
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	3	0.29
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	3	0.29
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	3	0.29
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	3	0.29
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	3	0.29
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	3	0.29
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	3	0.29
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	3	0.29
(1,2624)	1:173:A:GLU:HG2	1:172:A:GLU:H	9	0.29
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG11	8	0.29
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG12	8	0.29
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG13	8	0.29
(1,2436)	1:66:A:ILE:HG12	1:56:A:SER:H	4	0.29
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	3	0.29
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	3	0.29
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	3	0.29
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	7	0.29
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	7	0.29
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	7	0.29
(1,2277)	1:127:A:LYS:HA	1:127:A:LYS:HD3	6	0.29
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE1	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE2	5	0.29
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	2	0.29
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG11	10	0.29
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG12	10	0.29
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG13	10	0.29
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG21	2	0.29
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG22	2	0.29
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG23	2	0.29
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG21	2	0.29
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG22	2	0.29
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG23	2	0.29
(1,1984)	1:35:A:GLY:HA2	1:36:A:GLN:H	6	0.29
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	5	0.29
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	5	0.29
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	5	0.29
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	3	0.29
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	5	0.29
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE1	3	0.29
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE2	3	0.29
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG21	7	0.29
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG22	7	0.29
(1,1664)	1:143:A:GLN:H	1:177:A:THR:HG23	7	0.29
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	8	0.29
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG21	10	0.29
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG22	10	0.29
(1,1556)	1:41:A:ILE:H	1:42:A:ILE:HG23	10	0.29
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD11	8	0.29
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD12	8	0.29
(1,1446)	1:1:A:MET:HE1	1:9:A:LEU:HD13	8	0.29
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD11	8	0.29
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD12	8	0.29
(1,1446)	1:1:A:MET:HE2	1:9:A:LEU:HD13	8	0.29
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD11	8	0.29
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD12	8	0.29
(1,1446)	1:1:A:MET:HE3	1:9:A:LEU:HD13	8	0.29
(1,1403)	1:179:A:PHE:HD1	1:179:A:PHE:H	7	0.29
(1,1403)	1:179:A:PHE:HD2	1:179:A:PHE:H	7	0.29
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	4	0.29
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	4	0.29
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	4	0.29
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	4	0.29
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	4	0.29
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	4	0.29
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	4	0.29
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	4	0.29
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD11	2	0.29
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD12	2	0.29
(1,1323)	1:145:A:ILE:HB	1:145:A:ILE:HD13	2	0.29
(1,1312)	1:39:A:VAL:H	1:38:A:LEU:HD21	7	0.29
(1,1312)	1:39:A:VAL:H	1:38:A:LEU:HD22	7	0.29
(1,1312)	1:39:A:VAL:H	1:38:A:LEU:HD23	7	0.29
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD21	2	0.29
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD22	2	0.29
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD23	2	0.29
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	3	0.29
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	3	0.29
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	3	0.29
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	3	0.29
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	3	0.29
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	3	0.29
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	3	0.29
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	3	0.29
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	3	0.29
(1,1152)	1:62:A:ASN:HD22	1:63:A:ALA:H	3	0.29
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD21	3	0.29
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD22	3	0.29
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD23	3	0.29
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	7	0.29
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	3	0.29
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	3	0.29
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	3	0.29
(1,935)	1:125:A:ALA:HA	1:132:A:ILE:HB	5	0.29
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	3	0.29
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	3	0.29
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	3	0.29
(1,818)	1:114:A:GLY:H	1:115:A:MET:H	4	0.29
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	8	0.29
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	8	0.29
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD11	4	0.29
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD12	4	0.29
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD13	4	0.29
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	7	0.29
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	7	0.29
(1,670)	1:143:A:GLN:HG3	1:142:A:LEU:H	5	0.29
(1,645)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	6	0.29
(1,555)	1:155:A:GLN:HG2	1:156:A:GLN:HE22	5	0.29
(1,467)	1:122:A:CYS:HB3	1:134:A:HIS:H	1	0.29
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	2	0.29
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD11	3	0.29
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD12	3	0.29
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD13	3	0.29
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD21	3	0.29
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD22	3	0.29
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD23	3	0.29
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	10	0.29
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	10	0.29
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	10	0.29
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE1	8	0.29
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE2	8	0.29
(1,326)	2:201:A:Z90:HAT	1:115:A:MET:HE3	8	0.29
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	1	0.29
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	1	0.29
(1,312)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	1	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	1	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	2	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	3	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	4	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	5	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	6	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	7	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	8	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	9	0.29
(1,283)	2:201:A:Z90:HAE	2:201:A:Z90:HAJ	10	0.29
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG11	4	0.29
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG12	4	0.29
(1,275)	2:201:A:Z90:HAF	1:39:A:VAL:HG13	4	0.29
(1,269)	1:101:A:LEU:HD11	2:201:A:Z90:HAI	9	0.29
(1,269)	1:101:A:LEU:HD12	2:201:A:Z90:HAI	9	0.29
(1,269)	1:101:A:LEU:HD13	2:201:A:Z90:HAI	9	0.29
(1,160)	1:171:A:ASN:H	1:174:A:CYS:HB2	5	0.29
(1,160)	1:171:A:ASN:H	1:174:A:CYS:HB3	5	0.29
(1,3573)	1:22:A:TRP:HE3	1:26:A:LYS:HB2	8	0.28
(1,3459)	1:34:A:GLU:HB2	1:35:A:GLY:H	5	0.28
(1,3459)	1:34:A:GLU:HB3	1:35:A:GLY:H	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3443)	1:143:A:GLN:HG3	1:144:A:ASP:H	5	0.28
(1,3408)	1:140:A:GLU:HB3	1:169:A:GLN:HE22	10	0.28
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD11	8	0.28
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD12	8	0.28
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD13	8	0.28
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD11	8	0.28
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD12	8	0.28
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD13	8	0.28
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD11	8	0.28
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD12	8	0.28
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD13	8	0.28
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG11	9	0.28
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG12	9	0.28
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG13	9	0.28
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG21	9	0.28
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG22	9	0.28
(1,3321)	1:22:A:TRP:HH2	1:13:A:VAL:HG23	9	0.28
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD21	5	0.28
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD22	5	0.28
(1,3269)	1:37:A:PHE:HE1	1:31:A:LEU:HD23	5	0.28
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD21	5	0.28
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD22	5	0.28
(1,3269)	1:37:A:PHE:HE2	1:31:A:LEU:HD23	5	0.28
(1,3234)	1:100:A:ASN:HD22	1:96:A:GLU:HB3	4	0.28
(1,3083)	1:149:A:ILE:H	1:71:A:GLY:H	4	0.28
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	2	0.28
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	2	0.28
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	2	0.28
(1,2560)	1:141:A:GLY:HA3	1:144:A:ASP:H	6	0.28
(1,2466)	1:95:A:ARG:H	1:93:A:ASN:H	7	0.28
(1,2436)	1:66:A:ILE:HG12	1:56:A:SER:H	1	0.28
(1,2307)	1:173:A:GLU:H	1:173:A:GLU:HB2	1	0.28
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	7	0.28
(1,2200)	1:164:A:MET:HA	1:181:A:ILE:HA	10	0.28
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	8	0.28
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	10	0.28
(1,2130)	1:167:A:ILE:HG12	1:179:A:PHE:H	7	0.28
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	4	0.28
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG21	1	0.28
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG22	1	0.28
(1,2068)	1:17:A:TYR:H	1:21:A:VAL:HG23	1	0.28
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB1	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB2	3	0.28
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB3	3	0.28
(1,1984)	1:35:A:GLY:HA2	1:36:A:GLN:H	4	0.28
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG11	3	0.28
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG12	3	0.28
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG13	3	0.28
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG21	3	0.28
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG22	3	0.28
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG23	3	0.28
(1,1960)	1:184:A:LYS:HE2	1:184:A:LYS:HA	9	0.28
(1,1841)	1:92:A:SER:H	1:96:A:GLU:H	9	0.28
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	3	0.28
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	2	0.28
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	2	0.28
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	2	0.28
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	4	0.28
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	4	0.28
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	4	0.28
(1,1351)	1:184:A:LYS:HA	1:185:A:GLU:H	5	0.28
(1,1345)	1:19:A:PRO:HD2	1:18:A:GLY:H	7	0.28
(1,1335)	1:170:A:ARG:H	1:178:A:GLN:H	5	0.28
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD21	5	0.28
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD22	5	0.28
(1,1251)	1:31:A:LEU:H	1:51:A:LEU:HD23	5	0.28
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG11	9	0.28
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG12	9	0.28
(1,1242)	1:142:A:LEU:HD21	1:52:A:VAL:HG13	9	0.28
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG11	9	0.28
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG12	9	0.28
(1,1242)	1:142:A:LEU:HD22	1:52:A:VAL:HG13	9	0.28
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG11	9	0.28
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG12	9	0.28
(1,1242)	1:142:A:LEU:HD23	1:52:A:VAL:HG13	9	0.28
(1,1220)	1:23:A:GLU:HG2	1:20:A:GLU:HA	2	0.28
(1,1179)	1:167:A:ILE:HG12	1:179:A:PHE:H	8	0.28
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	6	0.28
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	6	0.28
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	6	0.28
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	6	0.28
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	6	0.28
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	6	0.28
(1,993)	1:169:A:GLN:HE22	1:169:A:GLN:H	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE1	10	0.28
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE2	10	0.28
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	6	0.28
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	6	0.28
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	6	0.28
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	6	0.28
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	6	0.28
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	6	0.28
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	6	0.28
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	6	0.28
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	6	0.28
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	10	0.28
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	10	0.28
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	10	0.28
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	10	0.28
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	10	0.28
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	10	0.28
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	10	0.28
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	10	0.28
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	10	0.28
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	4	0.28
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	6	0.28
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	6	0.28
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	6	0.28
(1,823)	1:183:A:GLU:HA	1:162:A:ILE:H	5	0.28
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD11	9	0.28
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD12	9	0.28
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD13	9	0.28
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	9	0.28
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	9	0.28
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	9	0.28
(1,647)	1:39:A:VAL:HB	1:40:A:ARG:H	3	0.28
(1,535)	1:129:A:LYS:HA	1:131:A:LEU:H	3	0.28
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	10	0.28
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	4	0.28
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG21	8	0.28
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG22	8	0.28
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG23	8	0.28
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG21	8	0.28
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG22	8	0.28
(1,336)	2:201:A:Z90:HAT	1:5:A:VAL:HG23	8	0.28
(1,334)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	9	0.28
(1,334)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	9	0.28
(1,308)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	3	0.28
(1,308)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	3	0.28
(1,308)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	3	0.28
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	4	0.28
(1,298)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	6	0.28
(1,287)	1:39:A:VAL:HG11	2:201:A:Z90:HAJ	1	0.28
(1,287)	1:39:A:VAL:HG12	2:201:A:Z90:HAJ	1	0.28
(1,287)	1:39:A:VAL:HG13	2:201:A:Z90:HAJ	1	0.28
(1,266)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	6	0.28
(1,266)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	6	0.28
(1,266)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	6	0.28
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	3	0.28
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG11	7	0.28
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG12	7	0.28
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG13	7	0.28
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG21	7	0.28
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG22	7	0.28
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG23	7	0.28
(1,17)	1:27:A:LYS:HD3	1:27:A:LYS:HB2	9	0.28
(1,17)	1:27:A:LYS:HD3	1:27:A:LYS:HB3	9	0.28
(1,3466)	1:93:A:ASN:HA	1:96:A:GLU:H	1	0.27
(1,3455)	1:95:A:ARG:HD2	1:96:A:GLU:H	10	0.27
(1,3455)	1:95:A:ARG:HD3	1:96:A:GLU:H	10	0.27
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	1	0.27
(1,3447)	1:66:A:ILE:HB	1:63:A:ALA:H	6	0.27
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD21	9	0.27
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD22	9	0.27
(1,3407)	1:143:A:GLN:H	1:142:A:LEU:HD23	9	0.27
(1,3401)	1:37:A:PHE:HD1	1:9:A:LEU:HD21	4	0.27
(1,3401)	1:37:A:PHE:HD1	1:9:A:LEU:HD22	4	0.27
(1,3401)	1:37:A:PHE:HD1	1:9:A:LEU:HD23	4	0.27
(1,3401)	1:37:A:PHE:HD2	1:9:A:LEU:HD21	4	0.27
(1,3401)	1:37:A:PHE:HD2	1:9:A:LEU:HD22	4	0.27
(1,3401)	1:37:A:PHE:HD2	1:9:A:LEU:HD23	4	0.27
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG21	1	0.27
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG22	1	0.27
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG23	1	0.27
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD21	6	0.27
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD22	6	0.27
(1,3249)	1:39:A:VAL:HG21	1:38:A:LEU:HD23	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD21	6	0.27
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD22	6	0.27
(1,3249)	1:39:A:VAL:HG22	1:38:A:LEU:HD23	6	0.27
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD21	6	0.27
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD22	6	0.27
(1,3249)	1:39:A:VAL:HG23	1:38:A:LEU:HD23	6	0.27
(1,3099)	1:8:A:ALA:HB1	1:12:A:LEU:H	3	0.27
(1,3099)	1:8:A:ALA:HB2	1:12:A:LEU:H	3	0.27
(1,3099)	1:8:A:ALA:HB3	1:12:A:LEU:H	3	0.27
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	5	0.27
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	5	0.27
(1,2758)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	5	0.27
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	5	0.27
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	5	0.27
(1,2758)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	5	0.27
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	5	0.27
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	5	0.27
(1,2758)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	5	0.27
(1,2720)	1:140:A:GLU:HG2	1:142:A:LEU:H	6	0.27
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG11	6	0.27
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG12	6	0.27
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG13	6	0.27
(1,2520)	1:93:A:ASN:HB2	1:94:A:VAL:H	2	0.27
(1,2520)	1:93:A:ASN:HB3	1:94:A:VAL:H	2	0.27
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD11	3	0.27
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD12	3	0.27
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD13	3	0.27
(1,2443)	1:94:A:VAL:HB	1:154:A:ALA:H	3	0.27
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD11	8	0.27
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD12	8	0.27
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD13	8	0.27
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	10	0.27
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	10	0.27
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	10	0.27
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD21	4	0.27
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD22	4	0.27
(1,2333)	1:77:A:PHE:HD1	1:11:A:LEU:HD23	4	0.27
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD21	4	0.27
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD22	4	0.27
(1,2333)	1:77:A:PHE:HD2	1:11:A:LEU:HD23	4	0.27
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	1	0.27
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG11	7	0.27
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG12	7	0.27
(1,2075)	1:143:A:GLN:HE22	1:166:A:VAL:HG13	7	0.27
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	1	0.27
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	1	0.27
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	1	0.27
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	1	0.27
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	1	0.27
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	1	0.27
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD11	9	0.27
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD12	9	0.27
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD13	9	0.27
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB1	10	0.27
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB2	10	0.27
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB3	10	0.27
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE1	5	0.27
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE2	5	0.27
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE3	5	0.27
(1,1774)	1:184:A:LYS:H	1:163:A:ASP:H	1	0.27
(1,1733)	1:49:A:TYR:HD1	1:142:A:LEU:H	4	0.27
(1,1733)	1:49:A:TYR:HD2	1:142:A:LEU:H	4	0.27
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	6	0.27
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	6	0.27
(1,1372)	1:124:A:ASP:HB2	1:125:A:ALA:H	10	0.27
(1,1345)	1:19:A:PRO:HD2	1:18:A:GLY:H	6	0.27
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	9	0.27
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	9	0.27
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	9	0.27
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	1	0.27
(1,1053)	1:162:A:ILE:HA	1:164:A:MET:H	2	0.27
(1,1026)	1:56:A:SER:HG	1:61:A:LEU:H	10	0.27
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	2	0.27
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD11	10	0.27
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD12	10	0.27
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD13	10	0.27
(1,864)	1:166:A:VAL:HB	1:178:A:GLN:H	2	0.27
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	3	0.27
(1,839)	1:133:A:LEU:HA	1:133:A:LEU:HD21	10	0.27
(1,839)	1:133:A:LEU:HA	1:133:A:LEU:HD22	10	0.27
(1,839)	1:133:A:LEU:HA	1:133:A:LEU:HD23	10	0.27
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	4	0.27
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD11	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD12	1	0.27
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD13	1	0.27
(1,810)	1:57:A:LYS:HG3	1:55:A:ALA:H	7	0.27
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	4	0.27
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	4	0.27
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	10	0.27
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	10	0.27
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	9	0.27
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	9	0.27
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	9	0.27
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	9	0.27
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	9	0.27
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	9	0.27
(1,649)	1:33:A:GLU:H	1:31:A:LEU:H	5	0.27
(1,601)	1:170:A:ARG:HG2	1:171:A:ASN:H	6	0.27
(1,596)	1:170:A:ARG:HG3	1:170:A:ARG:H	3	0.27
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE1	9	0.27
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE2	9	0.27
(1,565)	2:201:A:Z90:HAR	1:115:A:MET:HE3	9	0.27
(1,483)	1:10:A:GLU:HG3	1:22:A:TRP:HE1	2	0.27
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	3	0.27
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	7	0.27
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD11	5	0.27
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD12	5	0.27
(1,320)	2:201:A:Z90:HAP	1:104:A:LEU:HD13	5	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	2	0.27
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	2	0.27
(1,161)	1:171:A:ASN:HD22	1:171:A:ASN:H	8	0.27
(1,137)	1:56:A:SER:HB2	1:62:A:ASN:H	2	0.27
(1,137)	1:65:A:GLU:HA	1:62:A:ASN:H	9	0.27
(1,105)	1:182:A:GLU:H	1:164:A:MET:H	7	0.27
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE1	10	0.27
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE2	10	0.27
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE3	10	0.27
(1,9)	1:127:A:LYS:HA	1:126:A:GLU:HA	5	0.27
(1,3540)	1:54:A:ALA:HB1	1:28:A:GLU:H	3	0.26
(1,3540)	1:54:A:ALA:HB2	1:28:A:GLU:H	3	0.26
(1,3540)	1:54:A:ALA:HB3	1:28:A:GLU:H	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3535)	1:163:A:ASP:HB2	1:182:A:GLU:H	6	0.26
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG21	7	0.26
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG22	7	0.26
(1,3505)	1:157:A:ILE:HG21	1:153:A:VAL:HG23	7	0.26
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG21	7	0.26
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG22	7	0.26
(1,3505)	1:157:A:ILE:HG22	1:153:A:VAL:HG23	7	0.26
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG21	7	0.26
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG22	7	0.26
(1,3505)	1:157:A:ILE:HG23	1:153:A:VAL:HG23	7	0.26
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG21	8	0.26
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG22	8	0.26
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG23	8	0.26
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	9	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	2	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	2	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	2	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	5	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	5	0.26
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	5	0.26
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	1	0.26
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	1	0.26
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	1	0.26
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	1	0.26
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	1	0.26
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	1	0.26
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	3	0.26
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	3	0.26
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	3	0.26
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	3	0.26
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	3	0.26
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	3	0.26
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	6	0.26
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	6	0.26
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	6	0.26
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	6	0.26
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	6	0.26
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	6	0.26
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	10	0.26
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	10	0.26
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	10	0.26
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	10	0.26
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	10	0.26
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD21	8	0.26
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD22	8	0.26
(1,2883)	1:35:A:GLY:H	1:31:A:LEU:HD23	8	0.26
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD21	5	0.26
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD22	5	0.26
(1,2842)	1:71:A:GLY:H	1:67:A:LEU:HD23	5	0.26
(1,2640)	1:61:A:LEU:H	1:59:A:LEU:HG	6	0.26
(1,2560)	1:141:A:GLY:HA3	1:144:A:ASP:H	7	0.26
(1,2533)	1:69:A:MET:HE1	1:61:A:LEU:H	9	0.26
(1,2533)	1:69:A:MET:HE2	1:61:A:LEU:H	9	0.26
(1,2533)	1:69:A:MET:HE3	1:61:A:LEU:H	9	0.26
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	10	0.26
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	10	0.26
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	10	0.26
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD11	4	0.26
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD12	4	0.26
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD13	4	0.26
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	4	0.26
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	4	0.26
(1,2342)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	4	0.26
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	2	0.26
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE1	8	0.26
(1,2194)	1:142:A:LEU:HB2	1:49:A:TYR:HE2	8	0.26
(1,2158)	1:155:A:GLN:HG3	1:157:A:ILE:H	5	0.26
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	3	0.26
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	5	0.26
(1,2002)	1:174:A:CYS:H	1:173:A:GLU:HB3	5	0.26
(1,1960)	1:184:A:LYS:HE2	1:184:A:LYS:HA	7	0.26
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	3	0.26
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB1	5	0.26
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB2	5	0.26
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB3	5	0.26
(1,1601)	1:161:A:GLU:HG2	1:161:A:GLU:H	7	0.26
(1,1447)	1:146:A:VAL:HB	1:148:A:GLY:H	4	0.26
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG21	6	0.26
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG22	6	0.26
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG23	6	0.26
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG21	6	0.26
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG22	6	0.26
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG23	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG21	6	0.26
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG22	6	0.26
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG23	6	0.26
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	3	0.26
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	3	0.26
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	3	0.26
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	3	0.26
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	3	0.26
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	3	0.26
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	3	0.26
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	3	0.26
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	3	0.26
(1,1372)	1:124:A:ASP:HB2	1:125:A:ALA:H	2	0.26
(1,1238)	1:34:A:GLU:H	1:33:A:GLU:HB3	7	0.26
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD21	7	0.26
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD22	7	0.26
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD23	7	0.26
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	4	0.26
(1,948)	1:50:A:ASP:HB2	1:53:A:ALA:H	9	0.26
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD21	9	0.26
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD22	9	0.26
(1,931)	1:150:A:ILE:HD11	1:133:A:LEU:HD23	9	0.26
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD21	9	0.26
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD22	9	0.26
(1,931)	1:150:A:ILE:HD12	1:133:A:LEU:HD23	9	0.26
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD21	9	0.26
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD22	9	0.26
(1,931)	1:150:A:ILE:HD13	1:133:A:LEU:HD23	9	0.26
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	7	0.26
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	9	0.26
(1,798)	1:183:A:GLU:HA	1:162:A:ILE:HA	2	0.26
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD11	8	0.26
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD12	8	0.26
(1,779)	1:151:A:LYS:HA	1:162:A:ILE:HD13	8	0.26
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	1	0.26
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	1	0.26
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	1	0.26
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	7	0.26
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	7	0.26
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	7	0.26
(1,695)	1:76:A:VAL:HB	1:77:A:PHE:H	8	0.26
(1,670)	1:143:A:GLN:HG3	1:142:A:LEU:H	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:92:A:SER:H	1:96:A:GLU:HG2	10	0.26
(1,576)	1:171:A:ASN:H	1:169:A:GLN:HA	1	0.26
(1,564)	1:155:A:GLN:HG3	1:156:A:GLN:HE22	8	0.26
(1,535)	1:129:A:LYS:HA	1:131:A:LEU:H	7	0.26
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	5	0.26
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	8	0.26
(1,450)	1:155:A:GLN:HG3	1:159:A:GLY:H	2	0.26
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	7	0.26
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	8	0.26
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD11	9	0.26
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD12	9	0.26
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD13	9	0.26
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB1	3	0.26
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB2	3	0.26
(1,330)	2:201:A:Z90:HAR	1:117:A:ALA:HB3	3	0.26
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	4	0.26
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	4	0.26
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	4	0.26
(1,289)	1:149:A:ILE:HG21	2:201:A:Z90:HAI	7	0.26
(1,289)	1:149:A:ILE:HG22	2:201:A:Z90:HAI	7	0.26
(1,289)	1:149:A:ILE:HG23	2:201:A:Z90:HAI	7	0.26
(1,239)	1:69:A:MET:H	1:69:A:MET:HE1	6	0.26
(1,239)	1:69:A:MET:H	1:69:A:MET:HE2	6	0.26
(1,239)	1:69:A:MET:H	1:69:A:MET:HE3	6	0.26
(1,206)	1:180:A:LEU:HD11	1:131:A:LEU:H	4	0.26
(1,206)	1:180:A:LEU:HD12	1:131:A:LEU:H	4	0.26
(1,206)	1:180:A:LEU:HD13	1:131:A:LEU:H	4	0.26
(1,206)	1:180:A:LEU:HD21	1:131:A:LEU:H	4	0.26
(1,206)	1:180:A:LEU:HD22	1:131:A:LEU:H	4	0.26
(1,206)	1:180:A:LEU:HD23	1:131:A:LEU:H	4	0.26
(1,189)	1:43:A:TYR:HD1	1:6:A:ASN:H	3	0.26
(1,189)	1:43:A:TYR:HD2	1:6:A:ASN:H	3	0.26
(1,188)	1:165:A:LYS:HD2	1:166:A:VAL:H	4	0.26
(1,188)	1:165:A:LYS:HD3	1:166:A:VAL:H	4	0.26
(1,148)	1:145:A:ILE:HG12	1:143:A:GLN:H	8	0.26
(1,148)	1:145:A:ILE:HG13	1:143:A:GLN:H	8	0.26
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD11	6	0.26
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD12	6	0.26
(1,65)	1:145:A:ILE:HG21	1:67:A:LEU:HD13	6	0.26
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD11	6	0.26
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD12	6	0.26
(1,65)	1:145:A:ILE:HG22	1:67:A:LEU:HD13	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD11	6	0.26
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD12	6	0.26
(1,65)	1:145:A:ILE:HG23	1:67:A:LEU:HD13	6	0.26
(1,3495)	1:140:A:GLU:HA	1:143:A:GLN:H	10	0.25
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE1	9	0.25
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE2	9	0.25
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE3	9	0.25
(1,3353)	1:91:A:GLY:H	1:93:A:ASN:H	5	0.25
(1,3289)	1:63:A:ALA:HB1	1:67:A:LEU:H	2	0.25
(1,3289)	1:63:A:ALA:HB2	1:67:A:LEU:H	2	0.25
(1,3289)	1:63:A:ALA:HB3	1:67:A:LEU:H	2	0.25
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	2	0.25
(1,3100)	1:93:A:ASN:HD22	1:97:A:PHE:H	9	0.25
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	7	0.25
(1,3043)	1:57:A:LYS:H	1:25:A:ILE:HG12	6	0.25
(1,3043)	1:57:A:LYS:H	1:25:A:ILE:HG13	6	0.25
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	2	0.25
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	2	0.25
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	2	0.25
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	2	0.25
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	2	0.25
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	2	0.25
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	5	0.25
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	5	0.25
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	5	0.25
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	5	0.25
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	5	0.25
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	5	0.25
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	7	0.25
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	7	0.25
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	7	0.25
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	7	0.25
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	7	0.25
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	7	0.25
(1,3012)	1:176:A:HIS:H	1:174:A:CYS:HB3	10	0.25
(1,2786)	1:14:A:ILE:HG13	1:22:A:TRP:HE1	1	0.25
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG11	4	0.25
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG12	4	0.25
(1,2735)	1:1:A:MET:HE1	1:5:A:VAL:HG13	4	0.25
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG11	4	0.25
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG12	4	0.25
(1,2735)	1:1:A:MET:HE2	1:5:A:VAL:HG13	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG11	4	0.25
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG12	4	0.25
(1,2735)	1:1:A:MET:HE3	1:5:A:VAL:HG13	4	0.25
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	8	0.25
(1,2672)	1:179:A:PHE:HE1	1:146:A:VAL:H	4	0.25
(1,2672)	1:179:A:PHE:HE2	1:146:A:VAL:H	4	0.25
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB1	10	0.25
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB2	10	0.25
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB3	10	0.25
(1,2577)	1:128:A:GLY:HA3	1:130:A:GLY:H	3	0.25
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	8	0.25
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	8	0.25
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	8	0.25
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD11	9	0.25
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD12	9	0.25
(1,2344)	1:90:A:LEU:HA	1:90:A:LEU:HD13	9	0.25
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	8	0.25
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	9	0.25
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD11	6	0.25
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD12	6	0.25
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD13	6	0.25
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG12	8	0.25
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG13	8	0.25
(1,2118)	1:94:A:VAL:HG21	1:96:A:GLU:H	1	0.25
(1,2118)	1:94:A:VAL:HG22	1:96:A:GLU:H	1	0.25
(1,2118)	1:94:A:VAL:HG23	1:96:A:GLU:H	1	0.25
(1,2108)	1:16:A:ASN:HD22	1:12:A:LEU:HD11	3	0.25
(1,2108)	1:16:A:ASN:HD22	1:12:A:LEU:HD12	3	0.25
(1,2108)	1:16:A:ASN:HD22	1:12:A:LEU:HD13	3	0.25
(1,2108)	1:16:A:ASN:HD22	1:12:A:LEU:HD21	3	0.25
(1,2108)	1:16:A:ASN:HD22	1:12:A:LEU:HD22	3	0.25
(1,2108)	1:16:A:ASN:HD22	1:12:A:LEU:HD23	3	0.25
(1,2042)	1:176:A:HIS:H	1:174:A:CYS:H	2	0.25
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	2	0.25
(1,2017)	1:136:A:TYR:HB2	1:119:A:SER:H	5	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	4	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	4	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	4	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	4	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	4	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	4	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	6	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	6	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	6	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	6	0.25
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	6	0.25
(1,1984)	1:35:A:GLY:HA2	1:36:A:GLN:H	3	0.25
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD21	6	0.25
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD22	6	0.25
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD23	6	0.25
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD2	1	0.25
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD3	1	0.25
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	4	0.25
(1,1746)	1:100:A:ASN:HB2	1:103:A:ALA:H	8	0.25
(1,1693)	1:48:A:THR:HG1	1:48:A:THR:H	10	0.25
(1,1582)	1:164:A:MET:HE1	1:181:A:ILE:HB	10	0.25
(1,1582)	1:164:A:MET:HE2	1:181:A:ILE:HB	10	0.25
(1,1582)	1:164:A:MET:HE3	1:181:A:ILE:HB	10	0.25
(1,1502)	1:57:A:LYS:HG2	1:58:A:VAL:H	9	0.25
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	1	0.25
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	1	0.25
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	1	0.25
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	1	0.25
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	1	0.25
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	1	0.25
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	1	0.25
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	1	0.25
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	1	0.25
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD21	6	0.25
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD22	6	0.25
(1,1236)	1:145:A:ILE:HG13	1:142:A:LEU:HD23	6	0.25
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD11	2	0.25
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD12	2	0.25
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD13	2	0.25
(1,1146)	1:100:A:ASN:HD22	1:99:A:GLN:H	7	0.25
(1,1123)	1:94:A:VAL:HB	1:160:A:THR:HB	1	0.25
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	5	0.25
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	3	0.25
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	7	0.25
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	7	0.25
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	7	0.25
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD21	2	0.25
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD22	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:140:A:GLU:H	1:142:A:LEU:HD23	2	0.25
(1,971)	1:92:A:SER:HB3	1:93:A:ASN:H	8	0.25
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	2	0.25
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD11	9	0.25
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD12	9	0.25
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD13	9	0.25
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	1	0.25
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	1	0.25
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	1	0.25
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	10	0.25
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	10	0.25
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	10	0.25
(1,810)	1:57:A:LYS:HG3	1:55:A:ALA:H	2	0.25
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	2	0.25
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	2	0.25
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	2	0.25
(1,639)	1:38:A:LEU:HB3	1:41:A:ILE:H	7	0.25
(1,574)	1:120:A:PHE:H	1:121:A:ARG:HB3	7	0.25
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	1	0.25
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	3	0.25
(1,381)	1:100:A:ASN:H	1:99:A:GLN:H	7	0.25
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	4	0.25
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	4	0.25
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	4	0.25
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	4	0.25
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	4	0.25
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	4	0.25
(1,137)	1:56:A:SER:HB2	1:62:A:ASN:H	5	0.25
(1,69)	1:142:A:LEU:HD11	1:48:A:THR:HG21	4	0.25
(1,69)	1:142:A:LEU:HD11	1:48:A:THR:HG22	4	0.25
(1,69)	1:142:A:LEU:HD11	1:48:A:THR:HG23	4	0.25
(1,69)	1:142:A:LEU:HD12	1:48:A:THR:HG21	4	0.25
(1,69)	1:142:A:LEU:HD12	1:48:A:THR:HG22	4	0.25
(1,69)	1:142:A:LEU:HD12	1:48:A:THR:HG23	4	0.25
(1,69)	1:142:A:LEU:HD13	1:48:A:THR:HG21	4	0.25
(1,69)	1:142:A:LEU:HD13	1:48:A:THR:HG22	4	0.25
(1,69)	1:142:A:LEU:HD13	1:48:A:THR:HG23	4	0.25
(1,50)	1:65:A:GLU:HA	1:69:A:MET:HE1	10	0.25
(1,50)	1:65:A:GLU:HA	1:69:A:MET:HE2	10	0.25
(1,50)	1:65:A:GLU:HA	1:69:A:MET:HE3	10	0.25
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD11	8	0.25
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD12	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD13	8	0.25
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD21	8	0.25
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD22	8	0.25
(1,20)	1:180:A:LEU:HB2	1:180:A:LEU:HD23	8	0.25
(1,3584)	1:168:A:GLN:H	1:180:A:LEU:H	2	0.24
(1,3573)	1:22:A:TRP:HE3	1:26:A:LYS:HB2	2	0.24
(1,3506)	1:176:A:HIS:H	1:170:A:ARG:HG3	2	0.24
(1,3476)	1:150:A:ILE:HD11	1:98:A:LEU:HD11	4	0.24
(1,3476)	1:150:A:ILE:HD11	1:98:A:LEU:HD12	4	0.24
(1,3476)	1:150:A:ILE:HD11	1:98:A:LEU:HD13	4	0.24
(1,3476)	1:150:A:ILE:HD12	1:98:A:LEU:HD11	4	0.24
(1,3476)	1:150:A:ILE:HD12	1:98:A:LEU:HD12	4	0.24
(1,3476)	1:150:A:ILE:HD12	1:98:A:LEU:HD13	4	0.24
(1,3476)	1:150:A:ILE:HD13	1:98:A:LEU:HD11	4	0.24
(1,3476)	1:150:A:ILE:HD13	1:98:A:LEU:HD12	4	0.24
(1,3476)	1:150:A:ILE:HD13	1:98:A:LEU:HD13	4	0.24
(1,3284)	1:100:A:ASN:HB3	1:103:A:ALA:H	9	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD21	1	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD22	1	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD23	1	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD21	5	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD22	5	0.24
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD23	5	0.24
(1,3197)	1:139:A:ARG:HG2	1:140:A:GLU:H	2	0.24
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	2	0.24
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	2	0.24
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	2	0.24
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	6	0.24
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	6	0.24
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	6	0.24
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	8	0.24
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	8	0.24
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	8	0.24
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	8	0.24
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	8	0.24
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	8	0.24
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD11	1	0.24
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD12	1	0.24
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD13	1	0.24
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	2	0.24
(1,2873)	1:9:A:LEU:H	1:5:A:VAL:HG21	10	0.24
(1,2873)	1:9:A:LEU:H	1:5:A:VAL:HG22	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2873)	1:9:A:LEU:H	1:5:A:VAL:HG23	10	0.24
(1,2805)	1:26:A:LYS:HE3	1:22:A:TRP:HE1	1	0.24
(1,2734)	1:14:A:ILE:HB	1:16:A:ASN:H	6	0.24
(1,2712)	1:83:A:TYR:H	1:82:A:GLY:HA2	5	0.24
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	4	0.24
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	7	0.24
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	8	0.24
(1,2660)	1:184:A:LYS:HE3	1:184:A:LYS:H	2	0.24
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	4	0.24
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG21	5	0.24
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG22	5	0.24
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG23	5	0.24
(1,2624)	1:173:A:GLU:HG2	1:172:A:GLU:H	6	0.24
(1,2577)	1:128:A:GLY:HA3	1:130:A:GLY:H	9	0.24
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	4	0.24
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	4	0.24
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	4	0.24
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	5	0.24
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	5	0.24
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	5	0.24
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	5	0.24
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	5	0.24
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	5	0.24
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD21	3	0.24
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD22	3	0.24
(1,2399)	1:64:A:GLY:H	1:67:A:LEU:HD23	3	0.24
(1,2384)	1:115:A:MET:HE1	1:115:A:MET:HB3	2	0.24
(1,2384)	1:115:A:MET:HE2	1:115:A:MET:HB3	2	0.24
(1,2384)	1:115:A:MET:HE3	1:115:A:MET:HB3	2	0.24
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	2	0.24
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	7	0.24
(1,2192)	1:65:A:GLU:HG2	1:63:A:ALA:H	4	0.24
(1,2192)	1:65:A:GLU:HG3	1:63:A:ALA:H	4	0.24
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	1	0.24
(1,2171)	1:17:A:TYR:HD1	1:13:A:VAL:HA	2	0.24
(1,2171)	1:17:A:TYR:HD2	1:13:A:VAL:HA	2	0.24
(1,2118)	1:94:A:VAL:HG21	1:96:A:GLU:H	3	0.24
(1,2118)	1:94:A:VAL:HG22	1:96:A:GLU:H	3	0.24
(1,2118)	1:94:A:VAL:HG23	1:96:A:GLU:H	3	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	5	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	5	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	5	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	5	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	5	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	8	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	8	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	8	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	8	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	8	0.24
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	8	0.24
(1,1984)	1:35:A:GLY:HA2	1:36:A:GLN:H	9	0.24
(1,1901)	1:131:A:LEU:HG	1:131:A:LEU:H	2	0.24
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	6	0.24
(1,1842)	1:184:A:LYS:HA	1:184:A:LYS:HD2	8	0.24
(1,1842)	1:184:A:LYS:HA	1:184:A:LYS:HD3	8	0.24
(1,1742)	1:161:A:GLU:H	1:154:A:ALA:HB1	6	0.24
(1,1742)	1:161:A:GLU:H	1:154:A:ALA:HB2	6	0.24
(1,1742)	1:161:A:GLU:H	1:154:A:ALA:HB3	6	0.24
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD11	4	0.24
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD12	4	0.24
(1,1622)	1:52:A:VAL:HG21	1:66:A:ILE:HD13	4	0.24
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD11	4	0.24
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD12	4	0.24
(1,1622)	1:52:A:VAL:HG22	1:66:A:ILE:HD13	4	0.24
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD11	4	0.24
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD12	4	0.24
(1,1622)	1:52:A:VAL:HG23	1:66:A:ILE:HD13	4	0.24
(1,1575)	1:169:A:GLN:HE22	1:169:A:GLN:H	6	0.24
(1,1469)	1:171:A:ASN:HD22	1:171:A:ASN:HA	10	0.24
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	3	0.24
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	3	0.24
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	3	0.24
(1,1187)	1:31:A:LEU:HA	1:35:A:GLY:H	7	0.24
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	4	0.24
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	4	0.24
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	4	0.24
(1,1026)	1:56:A:SER:HG	1:61:A:LEU:H	6	0.24
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	1	0.24
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	3	0.24
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	3	0.24
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	3	0.24
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	3	0.24
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	3	0.24
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	3	0.24
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	3	0.24
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	3	0.24
(1,850)	1:140:A:GLU:HG2	1:141:A:GLY:H	3	0.24
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	7	0.24
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD11	10	0.24
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD12	10	0.24
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD13	10	0.24
(1,748)	1:143:A:GLN:HE22	1:141:A:GLY:H	1	0.24
(1,649)	1:33:A:GLU:H	1:31:A:LEU:H	1	0.24
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	2	0.24
(1,394)	1:16:A:ASN:HD22	1:12:A:LEU:HD11	3	0.24
(1,394)	1:16:A:ASN:HD22	1:12:A:LEU:HD12	3	0.24
(1,394)	1:16:A:ASN:HD22	1:12:A:LEU:HD13	3	0.24
(1,394)	1:16:A:ASN:HD22	1:12:A:LEU:HD21	3	0.24
(1,394)	1:16:A:ASN:HD22	1:12:A:LEU:HD22	3	0.24
(1,394)	1:16:A:ASN:HD22	1:12:A:LEU:HD23	3	0.24
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD11	4	0.24
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD12	4	0.24
(1,377)	1:42:A:ILE:HA	1:42:A:ILE:HD13	4	0.24
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	3	0.24
(1,272)	1:150:A:ILE:HD11	2:201:A:Z90:HAM	3	0.24
(1,272)	1:150:A:ILE:HD12	2:201:A:Z90:HAM	3	0.24
(1,272)	1:150:A:ILE:HD13	2:201:A:Z90:HAM	3	0.24
(1,261)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	8	0.24
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG21	1	0.24
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG22	1	0.24
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG23	1	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD11	1	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD12	1	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD13	1	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD21	1	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD22	1	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD23	1	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD11	6	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD12	6	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD13	6	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD21	6	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD22	6	0.24
(1,230)	1:125:A:ALA:H	1:131:A:LEU:HD23	6	0.24
(1,191)	1:43:A:TYR:HE1	1:43:A:TYR:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:43:A:TYR:HE2	1:43:A:TYR:H	5	0.24
(1,188)	1:165:A:LYS:HD2	1:166:A:VAL:H	3	0.24
(1,188)	1:165:A:LYS:HD3	1:166:A:VAL:H	3	0.24
(1,181)	1:40:A:ARG:HG2	1:40:A:ARG:H	6	0.24
(1,181)	1:40:A:ARG:HG3	1:40:A:ARG:H	6	0.24
(1,161)	1:171:A:ASN:HD22	1:171:A:ASN:H	7	0.24
(1,148)	1:145:A:ILE:HG12	1:143:A:GLN:H	3	0.24
(1,148)	1:145:A:ILE:HG13	1:143:A:GLN:H	3	0.24
(1,99)	1:125:A:ALA:HA	1:132:A:ILE:H	1	0.24
(1,99)	1:125:A:ALA:HA	1:132:A:ILE:H	5	0.24
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	1	0.24
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	1	0.24
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	1	0.24
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	1	0.24
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG21	10	0.23
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG22	10	0.23
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG23	10	0.23
(1,3443)	1:143:A:GLN:HG3	1:144:A:ASP:H	2	0.23
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG11	1	0.23
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG12	1	0.23
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG13	1	0.23
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG11	9	0.23
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG12	9	0.23
(1,3419)	1:94:A:VAL:H	1:94:A:VAL:HG13	9	0.23
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	9	0.23
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	9	0.23
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	9	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	3	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	3	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	3	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	5	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	5	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	5	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	9	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	9	0.23
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	9	0.23
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD11	2	0.23
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD12	2	0.23
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD13	2	0.23
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	7	0.23
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	1	0.23
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	1	0.23
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	3	0.23
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	3	0.23
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	3	0.23
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	3	0.23
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	9	0.23
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	6	0.23
(1,2681)	1:181:A:ILE:HB	1:183:A:GLU:H	5	0.23
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD11	3	0.23
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD12	3	0.23
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD13	3	0.23
(1,2271)	1:129:A:LYS:H	1:130:A:GLY:H	6	0.23
(1,2247)	1:174:A:CYS:H	1:174:A:CYS:HB3	1	0.23
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD11	7	0.23
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD12	7	0.23
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD13	7	0.23
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG12	1	0.23
(1,2184)	1:55:A:ALA:H	1:25:A:ILE:HG13	1	0.23
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	3	0.23
(1,2118)	1:94:A:VAL:HG21	1:96:A:GLU:H	5	0.23
(1,2118)	1:94:A:VAL:HG22	1:96:A:GLU:H	5	0.23
(1,2118)	1:94:A:VAL:HG23	1:96:A:GLU:H	5	0.23
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	10	0.23
(1,1988)	1:26:A:LYS:HB3	1:23:A:GLU:H	3	0.23
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	9	0.23
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	9	0.23
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	9	0.23
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	9	0.23
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	9	0.23
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	9	0.23
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD21	3	0.23
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD22	3	0.23
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD23	3	0.23
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	7	0.23
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	6	0.23
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD11	1	0.23
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD12	1	0.23
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD13	1	0.23
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD11	1	0.23
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD12	1	0.23
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD13	1	0.23
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD11	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD12	1	0.23
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD13	1	0.23
(1,1668)	1:104:A:LEU:HD21	1:101:A:LEU:HA	2	0.23
(1,1668)	1:104:A:LEU:HD22	1:101:A:LEU:HA	2	0.23
(1,1668)	1:104:A:LEU:HD23	1:101:A:LEU:HA	2	0.23
(1,1582)	1:164:A:MET:HE1	1:181:A:ILE:HB	7	0.23
(1,1582)	1:164:A:MET:HE2	1:181:A:ILE:HB	7	0.23
(1,1582)	1:164:A:MET:HE3	1:181:A:ILE:HB	7	0.23
(1,1554)	1:111:A:ILE:HD11	1:110:A:THR:H	10	0.23
(1,1554)	1:111:A:ILE:HD12	1:110:A:THR:H	10	0.23
(1,1554)	1:111:A:ILE:HD13	1:110:A:THR:H	10	0.23
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG21	9	0.23
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG22	9	0.23
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG23	9	0.23
(1,1502)	1:57:A:LYS:HG2	1:58:A:VAL:H	10	0.23
(1,1478)	1:49:A:TYR:HE1	1:142:A:LEU:HD11	2	0.23
(1,1478)	1:49:A:TYR:HE1	1:142:A:LEU:HD12	2	0.23
(1,1478)	1:49:A:TYR:HE1	1:142:A:LEU:HD13	2	0.23
(1,1478)	1:49:A:TYR:HE2	1:142:A:LEU:HD11	2	0.23
(1,1478)	1:49:A:TYR:HE2	1:142:A:LEU:HD12	2	0.23
(1,1478)	1:49:A:TYR:HE2	1:142:A:LEU:HD13	2	0.23
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	7	0.23
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	7	0.23
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	7	0.23
(1,1424)	1:99:A:GLN:HE22	1:96:A:GLU:HA	9	0.23
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG21	1	0.23
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG22	1	0.23
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG23	1	0.23
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG21	1	0.23
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG22	1	0.23
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG23	1	0.23
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG21	1	0.23
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG22	1	0.23
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG23	1	0.23
(1,1297)	1:145:A:ILE:HG12	1:71:A:GLY:H	1	0.23
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	9	0.23
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	9	0.23
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	9	0.23
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	9	0.23
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	9	0.23
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	9	0.23
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	9	0.23
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	9	0.23
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	6	0.23
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	6	0.23
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	6	0.23
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	6	0.23
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	6	0.23
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	6	0.23
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	6	0.23
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	6	0.23
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	6	0.23
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD11	5	0.23
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD12	5	0.23
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD13	5	0.23
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	2	0.23
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	2	0.23
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	2	0.23
(1,1152)	1:62:A:ASN:HD22	1:63:A:ALA:H	7	0.23
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	7	0.23
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	7	0.23
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	7	0.23
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD21	5	0.23
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD22	5	0.23
(1,901)	1:145:A:ILE:HD11	1:67:A:LEU:HD23	5	0.23
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD21	5	0.23
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD22	5	0.23
(1,901)	1:145:A:ILE:HD12	1:67:A:LEU:HD23	5	0.23
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD21	5	0.23
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD22	5	0.23
(1,901)	1:145:A:ILE:HD13	1:67:A:LEU:HD23	5	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD11	4	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD12	4	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD13	4	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD11	5	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD12	5	0.23
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD13	5	0.23
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE1	2	0.23
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE2	2	0.23
(1,879)	2:201:A:Z90:HAT	1:115:A:MET:HE3	2	0.23
(1,818)	1:114:A:GLY:H	1:115:A:MET:H	2	0.23
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	6	0.23
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:159:A:GLY:HA3	1:158:A:HIS:H	1	0.23
(1,710)	1:183:A:GLU:HG3	1:162:A:ILE:HG21	9	0.23
(1,710)	1:183:A:GLU:HG3	1:162:A:ILE:HG22	9	0.23
(1,710)	1:183:A:GLU:HG3	1:162:A:ILE:HG23	9	0.23
(1,630)	1:130:A:GLY:HA3	1:183:A:GLU:H	1	0.23
(1,444)	1:131:A:LEU:HG	1:132:A:ILE:H	1	0.23
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD11	5	0.23
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD12	5	0.23
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD13	5	0.23
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD21	5	0.23
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD22	5	0.23
(1,364)	1:69:A:MET:H	1:12:A:LEU:HD23	5	0.23
(1,334)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	7	0.23
(1,334)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	7	0.23
(1,334)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	7	0.23
(1,321)	1:104:A:LEU:HD11	2:201:A:Z90:HAM	5	0.23
(1,321)	1:104:A:LEU:HD12	2:201:A:Z90:HAM	5	0.23
(1,321)	1:104:A:LEU:HD13	2:201:A:Z90:HAM	5	0.23
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG21	8	0.23
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG22	8	0.23
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG23	8	0.23
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	1	0.23
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	1	0.23
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	1	0.23
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	1	0.23
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	1	0.23
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	1	0.23
(1,135)	1:59:A:LEU:HA	1:61:A:LEU:H	3	0.23
(1,120)	1:27:A:LYS:HD2	1:30:A:GLN:H	3	0.23
(1,120)	1:27:A:LYS:HD3	1:30:A:GLN:H	3	0.23
(1,9)	1:127:A:LYS:HA	1:128:A:GLY:HA2	7	0.23
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	5	0.23
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	5	0.23
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	5	0.23
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	5	0.23
(1,3506)	1:176:A:HIS:H	1:170:A:ARG:HG3	3	0.22
(1,3491)	1:95:A:ARG:HA	1:98:A:LEU:HD11	6	0.22
(1,3491)	1:95:A:ARG:HA	1:98:A:LEU:HD12	6	0.22
(1,3491)	1:95:A:ARG:HA	1:98:A:LEU:HD13	6	0.22
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	6	0.22
(1,3424)	1:77:A:PHE:HE1	1:11:A:LEU:HD11	7	0.22
(1,3424)	1:77:A:PHE:HE1	1:11:A:LEU:HD12	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3424)	1:77:A:PHE:HE1	1:11:A:LEU:HD13	7	0.22
(1,3424)	1:77:A:PHE:HE2	1:11:A:LEU:HD11	7	0.22
(1,3424)	1:77:A:PHE:HE2	1:11:A:LEU:HD12	7	0.22
(1,3424)	1:77:A:PHE:HE2	1:11:A:LEU:HD13	7	0.22
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	7	0.22
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	7	0.22
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	7	0.22
(1,3308)	1:27:A:LYS:HG3	1:28:A:GLU:H	6	0.22
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD21	8	0.22
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD22	8	0.22
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD23	8	0.22
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG21	2	0.22
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG22	2	0.22
(1,3206)	1:183:A:GLU:H	1:160:A:THR:HG23	2	0.22
(1,3149)	1:93:A:ASN:HA	1:95:A:ARG:H	7	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	5	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	5	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	5	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	8	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	8	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	8	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG21	10	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG22	10	0.22
(1,3128)	1:41:A:ILE:HG13	1:41:A:ILE:HG23	10	0.22
(1,2974)	1:116:A:ARG:HB2	1:117:A:ALA:H	9	0.22
(1,2974)	1:116:A:ARG:HB3	1:117:A:ALA:H	9	0.22
(1,2884)	1:131:A:LEU:HB3	1:130:A:GLY:H	10	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	3	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	3	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	3	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	3	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	3	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	3	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	7	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	7	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	7	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	7	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	7	0.22
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	7	0.22
(1,2720)	1:140:A:GLU:HG2	1:142:A:LEU:H	3	0.22
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	5	0.22
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	7	0.22
(1,2650)	1:172:A:GLU:H	1:173:A:GLU:H	8	0.22
(1,2640)	1:61:A:LEU:H	1:59:A:LEU:HG	9	0.22
(1,2513)	1:142:A:LEU:HD21	1:139:A:ARG:H	7	0.22
(1,2513)	1:142:A:LEU:HD22	1:139:A:ARG:H	7	0.22
(1,2513)	1:142:A:LEU:HD23	1:139:A:ARG:H	7	0.22
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD11	7	0.22
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD12	7	0.22
(1,2372)	1:9:A:LEU:HA	1:9:A:LEU:HD13	7	0.22
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	7	0.22
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	7	0.22
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	7	0.22
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	4	0.22
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	8	0.22
(1,2237)	1:120:A:PHE:HA	1:135:A:TYR:H	9	0.22
(1,2226)	1:161:A:GLU:HG3	1:161:A:GLU:H	7	0.22
(1,2171)	1:17:A:TYR:HD1	1:13:A:VAL:HA	10	0.22
(1,2171)	1:17:A:TYR:HD2	1:13:A:VAL:HA	10	0.22
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD11	7	0.22
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD12	7	0.22
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD13	7	0.22
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD21	7	0.22
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD22	7	0.22
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD23	7	0.22
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	4	0.22
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	4	0.22
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	4	0.22
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	3	0.22
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	10	0.22
(1,2101)	1:140:A:GLU:HB3	1:169:A:GLN:HE22	10	0.22
(1,2086)	1:93:A:ASN:HD22	1:96:A:GLU:H	6	0.22
(1,2083)	1:120:A:PHE:HE1	1:135:A:TYR:H	8	0.22
(1,2083)	1:120:A:PHE:HE2	1:135:A:TYR:H	8	0.22
(1,2015)	1:47:A:LYS:HE3	1:47:A:LYS:HA	7	0.22
(1,2002)	1:174:A:CYS:H	1:173:A:GLU:HB3	1	0.22
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	3	0.22
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	3	0.22
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	3	0.22
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD21	3	0.22
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD22	3	0.22
(1,1993)	1:69:A:MET:HE1	1:59:A:LEU:HD23	3	0.22
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD21	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD22	3	0.22
(1,1993)	1:69:A:MET:HE2	1:59:A:LEU:HD23	3	0.22
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD21	3	0.22
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD22	3	0.22
(1,1993)	1:69:A:MET:HE3	1:59:A:LEU:HD23	3	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG11	7	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG12	7	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG13	7	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG21	7	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG22	7	0.22
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG23	7	0.22
(1,1949)	1:175:A:ASP:H	1:170:A:ARG:HG3	6	0.22
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	7	0.22
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD2	6	0.22
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD3	6	0.22
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE1	7	0.22
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE2	7	0.22
(1,1807)	1:61:A:LEU:HB3	1:69:A:MET:HE3	7	0.22
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE1	7	0.22
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE2	7	0.22
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE3	7	0.22
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE1	9	0.22
(1,1773)	1:7:A:HIS:HD2	1:77:A:PHE:HE2	9	0.22
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	10	0.22
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	6	0.22
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	6	0.22
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	6	0.22
(1,1617)	1:49:A:TYR:HE1	1:48:A:THR:H	1	0.22
(1,1617)	1:49:A:TYR:HE2	1:48:A:THR:H	1	0.22
(1,1613)	1:24:A:ASP:HB3	1:21:A:VAL:H	6	0.22
(1,1586)	1:164:A:MET:HE1	1:162:A:ILE:HB	4	0.22
(1,1586)	1:164:A:MET:HE2	1:162:A:ILE:HB	4	0.22
(1,1586)	1:164:A:MET:HE3	1:162:A:ILE:HB	4	0.22
(1,1578)	1:99:A:GLN:HG2	1:101:A:LEU:H	10	0.22
(1,1502)	1:57:A:LYS:HG2	1:58:A:VAL:H	5	0.22
(1,1494)	1:176:A:HIS:H	1:174:A:CYS:HB2	3	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	1	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	1	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	1	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	8	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	8	0.22
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	9	0.22
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	9	0.22
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	9	0.22
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	9	0.22
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	9	0.22
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	9	0.22
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	9	0.22
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	9	0.22
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	9	0.22
(1,1271)	1:2:A:TYR:HD1	1:5:A:VAL:H	1	0.22
(1,1271)	1:2:A:TYR:HD2	1:5:A:VAL:H	1	0.22
(1,1264)	1:142:A:LEU:HD11	1:67:A:LEU:HD11	9	0.22
(1,1264)	1:142:A:LEU:HD11	1:67:A:LEU:HD12	9	0.22
(1,1264)	1:142:A:LEU:HD11	1:67:A:LEU:HD13	9	0.22
(1,1264)	1:142:A:LEU:HD12	1:67:A:LEU:HD11	9	0.22
(1,1264)	1:142:A:LEU:HD12	1:67:A:LEU:HD12	9	0.22
(1,1264)	1:142:A:LEU:HD12	1:67:A:LEU:HD13	9	0.22
(1,1264)	1:142:A:LEU:HD13	1:67:A:LEU:HD11	9	0.22
(1,1264)	1:142:A:LEU:HD13	1:67:A:LEU:HD12	9	0.22
(1,1264)	1:142:A:LEU:HD13	1:67:A:LEU:HD13	9	0.22
(1,1179)	1:167:A:ILE:HG12	1:179:A:PHE:H	7	0.22
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG21	4	0.22
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG22	4	0.22
(1,1173)	1:158:A:HIS:H	1:153:A:VAL:HG23	4	0.22
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	9	0.22
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	9	0.22
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	9	0.22
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	6	0.22
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE1	5	0.22
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE2	5	0.22
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE1	5	0.22
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE2	5	0.22
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE1	5	0.22
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE2	5	0.22
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD11	6	0.22
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD12	6	0.22
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD13	6	0.22
(1,874)	1:52:A:VAL:HB	1:67:A:LEU:H	6	0.22
(1,767)	1:66:A:ILE:HG12	1:61:A:LEU:H	4	0.22
(1,739)	1:48:A:THR:H	1:31:A:LEU:HD11	9	0.22
(1,739)	1:48:A:THR:H	1:31:A:LEU:HD12	9	0.22
(1,739)	1:48:A:THR:H	1:31:A:LEU:HD13	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	10	0.22
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	10	0.22
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	10	0.22
(1,670)	1:143:A:GLN:HG3	1:142:A:LEU:H	1	0.22
(1,619)	1:92:A:SER:H	1:96:A:GLU:HB3	7	0.22
(1,614)	1:170:A:ARG:HG2	1:170:A:ARG:H	10	0.22
(1,576)	1:171:A:ASN:H	1:169:A:GLN:HA	10	0.22
(1,488)	1:151:A:LYS:H	1:162:A:ILE:HG13	10	0.22
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	9	0.22
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE1	8	0.22
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE2	8	0.22
(1,337)	2:201:A:Z90:HAF	1:115:A:MET:HE3	8	0.22
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE1	7	0.22
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE2	7	0.22
(1,255)	2:201:A:Z90:HAR	1:115:A:MET:HE3	7	0.22
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD21	7	0.22
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD22	7	0.22
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD23	7	0.22
(1,198)	1:120:A:PHE:HA	1:135:A:TYR:H	9	0.22
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	4	0.22
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	4	0.22
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	7	0.22
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	7	0.22
(1,82)	1:19:A:PRO:HG2	1:21:A:VAL:H	2	0.22
(1,82)	1:19:A:PRO:HG3	1:21:A:VAL:H	2	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	2	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	2	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	2	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	2	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	3	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	3	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	3	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	3	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	4	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	4	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	4	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	4	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	6	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	6	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	6	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	6	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	7	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	7	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	7	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	8	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	8	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	8	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	8	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	9	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	9	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	9	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	9	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB2	10	0.22
(1,1)	1:113:A:PRO:HG2	1:113:A:PRO:HB3	10	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB2	10	0.22
(1,1)	1:113:A:PRO:HG3	1:113:A:PRO:HB3	10	0.22
(1,3540)	1:54:A:ALA:HB1	1:28:A:GLU:H	4	0.21
(1,3540)	1:54:A:ALA:HB2	1:28:A:GLU:H	4	0.21
(1,3540)	1:54:A:ALA:HB3	1:28:A:GLU:H	4	0.21
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	5	0.21
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	5	0.21
(1,3461)	1:132:A:ILE:HG12	1:125:A:ALA:H	2	0.21
(1,3444)	1:81:A:SER:H	1:83:A:TYR:HD1	5	0.21
(1,3444)	1:81:A:SER:H	1:83:A:TYR:HD2	5	0.21
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE1	2	0.21
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE2	2	0.21
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE3	2	0.21
(1,3354)	1:27:A:LYS:HD3	1:28:A:GLU:H	6	0.21
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	7	0.21
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	7	0.21
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	7	0.21
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	4	0.21
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	4	0.21
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	4	0.21
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	6	0.21
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	6	0.21
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	6	0.21
(1,3297)	1:143:A:GLN:HE22	1:142:A:LEU:H	6	0.21
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD21	2	0.21
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD22	2	0.21
(1,3228)	1:29:A:ALA:H	1:51:A:LEU:HD23	2	0.21
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	8	0.21
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	10	0.21
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	10	0.21
(1,2967)	1:160:A:THR:H	1:157:A:ILE:H	5	0.21
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	10	0.21
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	10	0.21
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	10	0.21
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	10	0.21
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	10	0.21
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	10	0.21
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	2	0.21
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	6	0.21
(1,2675)	1:60:A:ASN:HD22	1:60:A:ASN:HB2	8	0.21
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	2	0.21
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	2	0.21
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	2	0.21
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	4	0.21
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	4	0.21
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	4	0.21
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	7	0.21
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	7	0.21
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	7	0.21
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	4	0.21
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	4	0.21
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	4	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD11	3	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD12	3	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD13	3	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD21	3	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD22	3	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD23	3	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD11	4	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD12	4	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD13	4	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD21	4	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD22	4	0.21
(1,2154)	1:131:A:LEU:HB3	1:131:A:LEU:HD23	4	0.21
(1,2092)	1:132:A:ILE:HD11	1:131:A:LEU:H	7	0.21
(1,2092)	1:132:A:ILE:HD12	1:131:A:LEU:H	7	0.21
(1,2092)	1:132:A:ILE:HD13	1:131:A:LEU:H	7	0.21
(1,2015)	1:47:A:LYS:HE3	1:47:A:LYS:HA	9	0.21
(1,2005)	1:47:A:LYS:HE3	1:47:A:LYS:H	9	0.21
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	9	0.21
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	9	0.21
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD21	3	0.21
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD22	3	0.21
(1,1907)	1:7:A:HIS:HD2	1:11:A:LEU:HD23	3	0.21
(1,1901)	1:131:A:LEU:HG	1:131:A:LEU:H	9	0.21
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	10	0.21
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD11	8	0.21
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD12	8	0.21
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD13	8	0.21
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD11	8	0.21
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD12	8	0.21
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD13	8	0.21
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD11	8	0.21
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD12	8	0.21
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD13	8	0.21
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD11	4	0.21
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD12	4	0.21
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD13	4	0.21
(1,1731)	1:174:A:CYS:H	1:171:A:ASN:HB2	2	0.21
(1,1725)	1:128:A:GLY:H	1:130:A:GLY:H	3	0.21
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG11	1	0.21
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG12	1	0.21
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG13	1	0.21
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG11	1	0.21
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG12	1	0.21
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG13	1	0.21
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG11	1	0.21
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG12	1	0.21
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG13	1	0.21
(1,1617)	1:49:A:TYR:HE1	1:48:A:THR:H	3	0.21
(1,1617)	1:49:A:TYR:HE2	1:48:A:THR:H	3	0.21
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	10	0.21
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	10	0.21
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	10	0.21
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	10	0.21
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	10	0.21
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	10	0.21
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	10	0.21
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	10	0.21
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	10	0.21
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1444)	1:176:A:HIS:H	1:171:A:ASN:H	5	0.21
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	5	0.21
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	5	0.21
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	5	0.21
(1,1345)	1:19:A:PRO:HD2	1:18:A:GLY:H	8	0.21
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	2	0.21
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	4	0.21
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	4	0.21
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	4	0.21
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	4	0.21
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	4	0.21
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	4	0.21
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	4	0.21
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	4	0.21
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	4	0.21
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	7	0.21
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	7	0.21
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	7	0.21
(1,1138)	1:73:A:MET:HE1	1:16:A:ASN:H	1	0.21
(1,1138)	1:73:A:MET:HE2	1:16:A:ASN:H	1	0.21
(1,1138)	1:73:A:MET:HE3	1:16:A:ASN:H	1	0.21
(1,1093)	1:166:A:VAL:HB	1:180:A:LEU:H	3	0.21
(1,1090)	1:157:A:ILE:HG13	1:157:A:ILE:H	5	0.21
(1,1075)	1:51:A:LEU:HA	1:29:A:ALA:H	10	0.21
(1,998)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	5	0.21
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE1	9	0.21
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE2	9	0.21
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	4	0.21
(1,859)	1:14:A:ILE:HG12	1:15:A:ARG:H	2	0.21
(1,624)	1:92:A:SER:H	1:96:A:GLU:HG3	4	0.21
(1,548)	1:143:A:GLN:HE22	1:144:A:ASP:H	1	0.21
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	1	0.21
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	8	0.21
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	8	0.21
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	8	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	1	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	1	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	1	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	2	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	2	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	2	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	3	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	3	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	4	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	4	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	4	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	5	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	5	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	5	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	6	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	6	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	6	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	7	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	7	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	7	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	8	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	8	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	8	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	9	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	9	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	9	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG21	10	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG22	10	0.21
(1,384)	1:48:A:THR:HB	1:48:A:THR:HG23	10	0.21
(1,298)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	4	0.21
(1,195)	1:121:A:ARG:HG2	1:123:A:THR:H	1	0.21
(1,195)	1:121:A:ARG:HG3	1:123:A:THR:H	1	0.21
(1,135)	1:59:A:LEU:HA	1:61:A:LEU:H	9	0.21
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	6	0.21
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	6	0.21
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	6	0.21
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	6	0.21
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD11	3	0.21
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD12	3	0.21
(1,75)	1:29:A:ALA:HB1	1:9:A:LEU:HD13	3	0.21
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD11	3	0.21
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD12	3	0.21
(1,75)	1:29:A:ALA:HB2	1:9:A:LEU:HD13	3	0.21
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD11	3	0.21
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD12	3	0.21
(1,75)	1:29:A:ALA:HB3	1:9:A:LEU:HD13	3	0.21
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE1	4	0.21
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:11:A:LEU:HA	1:73:A:MET:HE3	4	0.21
(1,3466)	1:93:A:ASN:HA	1:96:A:GLU:H	2	0.2
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	10	0.2
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	6	0.2
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	6	0.2
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	6	0.2
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	6	0.2
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	6	0.2
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	6	0.2
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	6	0.2
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	6	0.2
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	6	0.2
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD11	10	0.2
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD12	10	0.2
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD13	10	0.2
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD11	1	0.2
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD12	1	0.2
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD13	1	0.2
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	10	0.2
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	10	0.2
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	10	0.2
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB1	7	0.2
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB2	7	0.2
(1,3192)	1:52:A:VAL:H	1:29:A:ALA:HB3	7	0.2
(1,3179)	1:158:A:HIS:HD2	1:158:A:HIS:H	9	0.2
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	2	0.2
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	9	0.2
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	7	0.2
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	8	0.2
(1,2961)	1:123:A:THR:HB	1:124:A:ASP:H	2	0.2
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	4	0.2
(1,2834)	1:170:A:ARG:H	1:177:A:THR:HG21	2	0.2
(1,2834)	1:170:A:ARG:H	1:177:A:THR:HG22	2	0.2
(1,2834)	1:170:A:ARG:H	1:177:A:THR:HG23	2	0.2
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	1	0.2
(1,2700)	1:120:A:PHE:HA	1:134:A:HIS:H	9	0.2
(1,2642)	1:61:A:LEU:HG	1:61:A:LEU:H	8	0.2
(1,2570)	1:26:A:LYS:HG3	1:22:A:TRP:HE1	2	0.2
(1,2556)	1:69:A:MET:HE1	1:59:A:LEU:HD21	4	0.2
(1,2556)	1:69:A:MET:HE1	1:59:A:LEU:HD22	4	0.2
(1,2556)	1:69:A:MET:HE1	1:59:A:LEU:HD23	4	0.2
(1,2556)	1:69:A:MET:HE2	1:59:A:LEU:HD21	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2556)	1:69:A:MET:HE2	1:59:A:LEU:HD22	4	0.2
(1,2556)	1:69:A:MET:HE2	1:59:A:LEU:HD23	4	0.2
(1,2556)	1:69:A:MET:HE3	1:59:A:LEU:HD21	4	0.2
(1,2556)	1:69:A:MET:HE3	1:59:A:LEU:HD22	4	0.2
(1,2556)	1:69:A:MET:HE3	1:59:A:LEU:HD23	4	0.2
(1,2552)	1:99:A:GLN:HE22	1:96:A:GLU:H	5	0.2
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG21	3	0.2
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG22	3	0.2
(1,2527)	1:56:A:SER:H	1:66:A:ILE:HG23	3	0.2
(1,2466)	1:95:A:ARG:H	1:93:A:ASN:H	5	0.2
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD11	9	0.2
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD12	9	0.2
(1,2444)	1:52:A:VAL:HB	1:9:A:LEU:HD13	9	0.2
(1,2394)	1:17:A:TYR:HE1	1:13:A:VAL:H	5	0.2
(1,2394)	1:17:A:TYR:HE2	1:13:A:VAL:H	5	0.2
(1,2384)	1:115:A:MET:HE1	1:115:A:MET:HB3	5	0.2
(1,2384)	1:115:A:MET:HE2	1:115:A:MET:HB3	5	0.2
(1,2384)	1:115:A:MET:HE3	1:115:A:MET:HB3	5	0.2
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	1	0.2
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	1	0.2
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	1	0.2
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD11	4	0.2
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD12	4	0.2
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD13	4	0.2
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD21	4	0.2
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD22	4	0.2
(1,2341)	1:112:A:TYR:HE1	1:108:A:LEU:HD23	4	0.2
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD11	4	0.2
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD12	4	0.2
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD13	4	0.2
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD21	4	0.2
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD22	4	0.2
(1,2341)	1:112:A:TYR:HE2	1:108:A:LEU:HD23	4	0.2
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	5	0.2
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	10	0.2
(1,2155)	1:125:A:ALA:HA	1:126:A:GLU:H	6	0.2
(1,2155)	1:125:A:ALA:HA	1:126:A:GLU:H	8	0.2
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	6	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	2	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	2	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	2	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	8	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	8	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	10	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	10	0.2
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	10	0.2
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG11	7	0.2
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG12	7	0.2
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG13	7	0.2
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG21	7	0.2
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG22	7	0.2
(1,1987)	1:22:A:TRP:HE3	1:13:A:VAL:HG23	7	0.2
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG11	9	0.2
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG12	9	0.2
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG13	9	0.2
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG21	9	0.2
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG22	9	0.2
(1,1980)	1:13:A:VAL:H	1:13:A:VAL:HG23	9	0.2
(1,1960)	1:184:A:LYS:HE2	1:184:A:LYS:HA	10	0.2
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	1	0.2
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD11	9	0.2
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD12	9	0.2
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD13	9	0.2
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB2	3	0.2
(1,1813)	1:116:A:ARG:HE	1:116:A:ARG:HB3	3	0.2
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	7	0.2
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	6	0.2
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD11	5	0.2
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD12	5	0.2
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD13	5	0.2
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD21	5	0.2
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD22	5	0.2
(1,1570)	1:115:A:MET:HE1	1:108:A:LEU:HD23	5	0.2
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD11	5	0.2
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD12	5	0.2
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD13	5	0.2
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD21	5	0.2
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD22	5	0.2
(1,1570)	1:115:A:MET:HE2	1:108:A:LEU:HD23	5	0.2
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD11	5	0.2
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD12	5	0.2
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD13	5	0.2
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD21	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD22	5	0.2
(1,1570)	1:115:A:MET:HE3	1:108:A:LEU:HD23	5	0.2
(1,1529)	1:93:A:ASN:HD22	1:93:A:ASN:H	6	0.2
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD11	5	0.2
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD12	5	0.2
(1,1522)	1:149:A:ILE:H	1:150:A:ILE:HD13	5	0.2
(1,1469)	1:171:A:ASN:HD22	1:171:A:ASN:HA	2	0.2
(1,1463)	1:143:A:GLN:HG3	1:166:A:VAL:HG11	8	0.2
(1,1463)	1:143:A:GLN:HG3	1:166:A:VAL:HG12	8	0.2
(1,1463)	1:143:A:GLN:HG3	1:166:A:VAL:HG13	8	0.2
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	10	0.2
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	10	0.2
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	10	0.2
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	10	0.2
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	10	0.2
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	10	0.2
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	10	0.2
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	10	0.2
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	10	0.2
(1,1298)	1:115:A:MET:HB3	1:117:A:ALA:H	3	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD11	6	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD12	6	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD13	6	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD11	6	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD12	6	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD13	6	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD11	7	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD12	7	0.2
(1,1296)	1:49:A:TYR:HD1	1:142:A:LEU:HD13	7	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD11	7	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD12	7	0.2
(1,1296)	1:49:A:TYR:HD2	1:142:A:LEU:HD13	7	0.2
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	2	0.2
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	2	0.2
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	2	0.2
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	2	0.2
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	2	0.2
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	2	0.2
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	2	0.2
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	2	0.2
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	2	0.2
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG11	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG12	8	0.2
(1,1161)	1:155:A:GLN:H	1:153:A:VAL:HG13	8	0.2
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	6	0.2
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	6	0.2
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	6	0.2
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG21	3	0.2
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG22	3	0.2
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG23	3	0.2
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	7	0.2
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	10	0.2
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	10	0.2
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	10	0.2
(1,1011)	1:169:A:GLN:HE22	1:169:A:GLN:H	2	0.2
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD11	1	0.2
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD12	1	0.2
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD13	1	0.2
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	3	0.2
(1,849)	1:112:A:TYR:HD1	1:111:A:ILE:HG21	3	0.2
(1,849)	1:112:A:TYR:HD1	1:111:A:ILE:HG22	3	0.2
(1,849)	1:112:A:TYR:HD1	1:111:A:ILE:HG23	3	0.2
(1,849)	1:112:A:TYR:HD2	1:111:A:ILE:HG21	3	0.2
(1,849)	1:112:A:TYR:HD2	1:111:A:ILE:HG22	3	0.2
(1,849)	1:112:A:TYR:HD2	1:111:A:ILE:HG23	3	0.2
(1,818)	1:114:A:GLY:H	1:115:A:MET:H	3	0.2
(1,780)	1:17:A:TYR:HE1	1:18:A:GLY:H	2	0.2
(1,780)	1:17:A:TYR:HE2	1:18:A:GLY:H	2	0.2
(1,761)	1:159:A:GLY:HA3	1:158:A:HIS:H	2	0.2
(1,697)	1:127:A:LYS:HA	1:128:A:GLY:HA3	7	0.2
(1,601)	1:170:A:ARG:HG2	1:171:A:ASN:H	2	0.2
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	3	0.2
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD2	5	0.2
(1,475)	1:94:A:VAL:HB	1:95:A:ARG:HD3	5	0.2
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG21	10	0.2
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG22	10	0.2
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG23	10	0.2
(1,396)	1:183:A:GLU:HB3	1:160:A:THR:HG21	10	0.2
(1,396)	1:183:A:GLU:HB3	1:160:A:THR:HG22	10	0.2
(1,396)	1:183:A:GLU:HB3	1:160:A:THR:HG23	10	0.2
(1,300)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	1	0.2
(1,300)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	4	0.2
(1,300)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	5	0.2
(1,300)	2:201:A:Z90:HAP	2:201:A:Z90:HBD	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	5	0.2
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	5	0.2
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	5	0.2
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	5	0.2
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	5	0.2
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	5	0.2
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	3	0.2
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	3	0.2
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	3	0.19
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	3	0.19
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	10	0.19
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	10	0.19
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD21	5	0.19
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD22	5	0.19
(1,3464)	2:201:A:Z90:HAP	1:101:A:LEU:HD23	5	0.19
(1,3408)	1:140:A:GLU:HB3	1:169:A:GLN:HE22	7	0.19
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG11	9	0.19
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG12	9	0.19
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG13	9	0.19
(1,3289)	1:63:A:ALA:HB1	1:67:A:LEU:H	3	0.19
(1,3289)	1:63:A:ALA:HB2	1:67:A:LEU:H	3	0.19
(1,3289)	1:63:A:ALA:HB3	1:67:A:LEU:H	3	0.19
(1,3278)	1:93:A:ASN:HA	1:97:A:PHE:H	4	0.19
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	9	0.19
(1,3039)	1:32:A:ASP:HB3	1:27:A:LYS:HA	3	0.19
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD11	6	0.19
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD12	6	0.19
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD13	6	0.19
(1,2886)	1:134:A:HIS:HD2	1:134:A:HIS:H	8	0.19
(1,2780)	1:26:A:LYS:HG3	1:22:A:TRP:HE1	6	0.19
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	2	0.19
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	2	0.19
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	2	0.19
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	2	0.19
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	2	0.19
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	2	0.19
(1,2701)	1:99:A:GLN:HE22	1:95:A:ARG:HG3	4	0.19
(1,2678)	1:127:A:LYS:HG2	1:129:A:LYS:H	9	0.19
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG11	1	0.19
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG12	1	0.19
(1,2598)	1:67:A:LEU:HA	1:52:A:VAL:HG13	1	0.19
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	1	0.19
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	1	0.19
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	5	0.19
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	5	0.19
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	5	0.19
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG21	9	0.19
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG22	9	0.19
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG23	9	0.19
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	7	0.19
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	7	0.19
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	7	0.19
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	7	0.19
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	7	0.19
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	7	0.19
(1,2408)	1:113:A:PRO:HA	1:115:A:MET:H	1	0.19
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	5	0.19
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	5	0.19
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	5	0.19
(1,2352)	1:111:A:ILE:HA	1:111:A:ILE:HG21	10	0.19
(1,2352)	1:111:A:ILE:HA	1:111:A:ILE:HG22	10	0.19
(1,2352)	1:111:A:ILE:HA	1:111:A:ILE:HG23	10	0.19
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB1	4	0.19
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB2	4	0.19
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB3	4	0.19
(1,2245)	1:27:A:LYS:HD3	1:28:A:GLU:H	1	0.19
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	4	0.19
(1,2171)	1:17:A:TYR:HD1	1:13:A:VAL:HA	4	0.19
(1,2171)	1:17:A:TYR:HD2	1:13:A:VAL:HA	4	0.19
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	1	0.19
(1,2042)	1:176:A:HIS:H	1:174:A:CYS:H	8	0.19
(1,2019)	1:83:A:TYR:H	1:83:A:TYR:HD1	10	0.19
(1,2019)	1:83:A:TYR:H	1:83:A:TYR:HD2	10	0.19
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	1	0.19
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	1	0.19
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	1	0.19
(1,1975)	1:129:A:LYS:H	1:128:A:GLY:H	5	0.19
(1,1817)	1:66:A:ILE:HB	1:56:A:SER:H	6	0.19
(1,1817)	1:66:A:ILE:HB	1:56:A:SER:H	9	0.19
(1,1693)	1:48:A:THR:HG1	1:48:A:THR:H	5	0.19
(1,1642)	1:183:A:GLU:HB3	1:163:A:ASP:H	8	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	1	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	1	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	2	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	2	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	2	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	4	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	4	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	4	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	8	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	8	0.19
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	8	0.19
(1,1583)	1:123:A:THR:HB	1:125:A:ALA:H	2	0.19
(1,1515)	1:142:A:LEU:H	1:142:A:LEU:HD11	9	0.19
(1,1515)	1:142:A:LEU:H	1:142:A:LEU:HD12	9	0.19
(1,1515)	1:142:A:LEU:H	1:142:A:LEU:HD13	9	0.19
(1,1472)	1:104:A:LEU:HD21	2:201:A:Z90:HAP	2	0.19
(1,1472)	1:104:A:LEU:HD22	2:201:A:Z90:HAP	2	0.19
(1,1472)	1:104:A:LEU:HD23	2:201:A:Z90:HAP	2	0.19
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD11	1	0.19
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD12	1	0.19
(1,1465)	1:73:A:MET:HE1	1:11:A:LEU:HD13	1	0.19
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD11	1	0.19
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD12	1	0.19
(1,1465)	1:73:A:MET:HE2	1:11:A:LEU:HD13	1	0.19
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD11	1	0.19
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD12	1	0.19
(1,1465)	1:73:A:MET:HE3	1:11:A:LEU:HD13	1	0.19
(1,1451)	1:4:A:PHE:H	1:39:A:VAL:HG21	2	0.19
(1,1451)	1:4:A:PHE:H	1:39:A:VAL:HG22	2	0.19
(1,1451)	1:4:A:PHE:H	1:39:A:VAL:HG23	2	0.19
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	2	0.19
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	2	0.19
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	2	0.19
(1,1335)	1:170:A:ARG:H	1:178:A:GLN:H	8	0.19
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	8	0.19
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	8	0.19
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	8	0.19
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	8	0.19
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	8	0.19
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	8	0.19
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	8	0.19
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	8	0.19
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG21	6	0.19
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG22	6	0.19
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG23	6	0.19
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB1	7	0.19
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB2	7	0.19
(1,1213)	1:50:A:ASP:H	1:29:A:ALA:HB3	7	0.19
(1,1152)	1:62:A:ASN:HD22	1:63:A:ALA:H	8	0.19
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD11	6	0.19
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD12	6	0.19
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD13	6	0.19
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD11	6	0.19
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD12	6	0.19
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD13	6	0.19
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	8	0.19
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	8	0.19
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	8	0.19
(1,1035)	1:170:A:ARG:HE	1:170:A:ARG:HG3	7	0.19
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD11	5	0.19
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD12	5	0.19
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD13	5	0.19
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD11	1	0.19
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD12	1	0.19
(1,889)	1:11:A:LEU:HA	1:11:A:LEU:HD13	1	0.19
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	1	0.19
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD21	4	0.19
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD22	4	0.19
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD23	4	0.19
(1,657)	1:31:A:LEU:HB3	1:33:A:GLU:H	9	0.19
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG21	10	0.19
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG22	10	0.19
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG23	10	0.19
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	2	0.19
(1,449)	1:18:A:GLY:H	1:21:A:VAL:HG11	2	0.19
(1,449)	1:18:A:GLY:H	1:21:A:VAL:HG12	2	0.19
(1,449)	1:18:A:GLY:H	1:21:A:VAL:HG13	2	0.19
(1,444)	1:131:A:LEU:HG	1:132:A:ILE:H	5	0.19
(1,353)	1:176:A:HIS:H	1:170:A:ARG:HG2	9	0.19
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	8	0.19
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	8	0.19
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	8	0.19
(1,319)	1:101:A:LEU:HD21	2:201:A:Z90:HAI	8	0.19
(1,319)	1:101:A:LEU:HD22	2:201:A:Z90:HAI	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:101:A:LEU:HD23	2:201:A:Z90:HAI	8	0.19
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD21	2	0.19
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD22	2	0.19
(1,314)	2:201:A:Z90:HAP	1:90:A:LEU:HD23	2	0.19
(1,266)	1:150:A:ILE:HD11	2:201:A:Z90:HAH	3	0.19
(1,266)	1:150:A:ILE:HD12	2:201:A:Z90:HAH	3	0.19
(1,266)	1:150:A:ILE:HD13	2:201:A:Z90:HAH	3	0.19
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	1	0.19
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	1	0.19
(1,259)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	1	0.19
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG12	8	0.19
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG13	8	0.19
(1,160)	1:171:A:ASN:H	1:174:A:CYS:HB2	8	0.19
(1,160)	1:171:A:ASN:H	1:174:A:CYS:HB3	8	0.19
(1,83)	1:23:A:GLU:HB2	1:22:A:TRP:H	1	0.19
(1,83)	1:23:A:GLU:HB3	1:22:A:TRP:H	1	0.19
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG21	4	0.18
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG22	4	0.18
(1,3525)	1:9:A:LEU:H	1:5:A:VAL:HG23	4	0.18
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG21	1	0.18
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG22	1	0.18
(1,3492)	1:124:A:ASP:H	1:123:A:THR:HG23	1	0.18
(1,3447)	1:66:A:ILE:HB	1:63:A:ALA:H	5	0.18
(1,3399)	1:24:A:ASP:HB3	1:21:A:VAL:HG11	10	0.18
(1,3399)	1:24:A:ASP:HB3	1:21:A:VAL:HG12	10	0.18
(1,3399)	1:24:A:ASP:HB3	1:21:A:VAL:HG13	10	0.18
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	6	0.18
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	6	0.18
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	6	0.18
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD11	2	0.18
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD12	2	0.18
(1,3152)	1:143:A:GLN:H	1:142:A:LEU:HD13	2	0.18
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	4	0.18
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD11	6	0.18
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD12	6	0.18
(1,3054)	1:62:A:ASN:H	1:61:A:LEU:HD13	6	0.18
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG21	4	0.18
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG22	4	0.18
(1,3047)	1:94:A:VAL:HB	1:157:A:ILE:HG23	4	0.18
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD11	10	0.18
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD12	10	0.18
(1,2965)	1:60:A:ASN:H	1:66:A:ILE:HD13	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2819)	1:160:A:THR:HB	1:159:A:GLY:H	8	0.18
(1,2781)	1:9:A:LEU:HD21	1:13:A:VAL:H	4	0.18
(1,2781)	1:9:A:LEU:HD22	1:13:A:VAL:H	4	0.18
(1,2781)	1:9:A:LEU:HD23	1:13:A:VAL:H	4	0.18
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	5	0.18
(1,2675)	1:60:A:ASN:HD22	1:60:A:ASN:HB2	9	0.18
(1,2673)	1:34:A:GLU:HA	1:35:A:GLY:H	8	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	6	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	6	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	6	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	7	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	7	0.18
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	7	0.18
(1,2436)	1:66:A:ILE:HG12	1:56:A:SER:H	7	0.18
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB1	4	0.18
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB2	4	0.18
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB3	4	0.18
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	3	0.18
(1,2273)	1:11:A:LEU:HB3	1:8:A:ALA:H	2	0.18
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	5	0.18
(1,2171)	1:17:A:TYR:HD1	1:13:A:VAL:HA	8	0.18
(1,2171)	1:17:A:TYR:HD2	1:13:A:VAL:HA	8	0.18
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	9	0.18
(1,2129)	1:99:A:GLN:H	1:98:A:LEU:H	4	0.18
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG21	8	0.18
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG22	8	0.18
(1,2036)	1:17:A:TYR:HE1	1:21:A:VAL:HG23	8	0.18
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG21	8	0.18
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG22	8	0.18
(1,2036)	1:17:A:TYR:HE2	1:21:A:VAL:HG23	8	0.18
(1,2011)	1:30:A:GLN:HE22	1:30:A:GLN:HA	4	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	5	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	5	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	5	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	6	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	6	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	6	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	7	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	7	0.18
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	7	0.18
(1,1988)	1:26:A:LYS:HB3	1:23:A:GLU:H	8	0.18
(1,1985)	1:136:A:TYR:HD1	1:135:A:TYR:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1985)	1:136:A:TYR:HD2	1:135:A:TYR:H	3	0.18
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG21	4	0.18
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG22	4	0.18
(1,1978)	1:95:A:ARG:H	1:160:A:THR:HG23	4	0.18
(1,1897)	1:19:A:PRO:HB2	1:21:A:VAL:H	8	0.18
(1,1842)	1:184:A:LYS:HA	1:184:A:LYS:HD2	6	0.18
(1,1842)	1:184:A:LYS:HA	1:184:A:LYS:HD3	6	0.18
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB1	4	0.18
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB2	4	0.18
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB3	4	0.18
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	8	0.18
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD11	8	0.18
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD12	8	0.18
(1,1815)	1:151:A:LYS:HA	1:162:A:ILE:HD13	8	0.18
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	5	0.18
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	5	0.18
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	5	0.18
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	7	0.18
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	7	0.18
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	7	0.18
(1,1627)	1:158:A:HIS:H	1:155:A:GLN:H	5	0.18
(1,1603)	1:176:A:HIS:H	1:170:A:ARG:H	5	0.18
(1,1582)	1:164:A:MET:HE1	1:181:A:ILE:HB	2	0.18
(1,1582)	1:164:A:MET:HE2	1:181:A:ILE:HB	2	0.18
(1,1582)	1:164:A:MET:HE3	1:181:A:ILE:HB	2	0.18
(1,1579)	1:58:A:VAL:H	1:59:A:LEU:HD11	2	0.18
(1,1579)	1:58:A:VAL:H	1:59:A:LEU:HD12	2	0.18
(1,1579)	1:58:A:VAL:H	1:59:A:LEU:HD13	2	0.18
(1,1532)	1:8:A:ALA:HB1	1:11:A:LEU:HD21	3	0.18
(1,1532)	1:8:A:ALA:HB1	1:11:A:LEU:HD22	3	0.18
(1,1532)	1:8:A:ALA:HB1	1:11:A:LEU:HD23	3	0.18
(1,1532)	1:8:A:ALA:HB2	1:11:A:LEU:HD21	3	0.18
(1,1532)	1:8:A:ALA:HB2	1:11:A:LEU:HD22	3	0.18
(1,1532)	1:8:A:ALA:HB2	1:11:A:LEU:HD23	3	0.18
(1,1532)	1:8:A:ALA:HB3	1:11:A:LEU:HD21	3	0.18
(1,1532)	1:8:A:ALA:HB3	1:11:A:LEU:HD22	3	0.18
(1,1532)	1:8:A:ALA:HB3	1:11:A:LEU:HD23	3	0.18
(1,1529)	1:93:A:ASN:HD22	1:93:A:ASN:H	2	0.18
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG21	8	0.18
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG22	8	0.18
(1,1421)	1:149:A:ILE:HG21	1:150:A:ILE:HG23	8	0.18
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG21	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG22	8	0.18
(1,1421)	1:149:A:ILE:HG22	1:150:A:ILE:HG23	8	0.18
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG21	8	0.18
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG22	8	0.18
(1,1421)	1:149:A:ILE:HG23	1:150:A:ILE:HG23	8	0.18
(1,1409)	1:14:A:ILE:HB	1:18:A:GLY:H	2	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	3	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	3	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	3	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	10	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	10	0.18
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	10	0.18
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG21	4	0.18
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG22	4	0.18
(1,1336)	1:94:A:VAL:HB	1:157:A:ILE:HG23	4	0.18
(1,1271)	1:2:A:TYR:HD1	1:5:A:VAL:H	3	0.18
(1,1271)	1:2:A:TYR:HD2	1:5:A:VAL:H	3	0.18
(1,1262)	1:176:A:HIS:H	1:170:A:ARG:HB2	7	0.18
(1,1262)	1:176:A:HIS:H	1:170:A:ARG:HB3	7	0.18
(1,1262)	1:176:A:HIS:H	1:170:A:ARG:HB2	9	0.18
(1,1262)	1:176:A:HIS:H	1:170:A:ARG:HB3	9	0.18
(1,1163)	1:153:A:VAL:HG11	1:153:A:VAL:H	4	0.18
(1,1163)	1:153:A:VAL:HG12	1:153:A:VAL:H	4	0.18
(1,1163)	1:153:A:VAL:HG13	1:153:A:VAL:H	4	0.18
(1,1124)	1:160:A:THR:HA	1:184:A:LYS:H	4	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	4	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	4	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	4	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	5	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	5	0.18
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	5	0.18
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	10	0.18
(1,948)	1:50:A:ASP:HB2	1:53:A:ALA:H	6	0.18
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	9	0.18
(1,892)	1:172:A:GLU:H	1:171:A:ASN:HD22	7	0.18
(1,837)	1:157:A:ILE:HG12	1:158:A:HIS:H	2	0.18
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD21	3	0.18
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD22	3	0.18
(1,791)	1:60:A:ASN:H	1:61:A:LEU:HD23	3	0.18
(1,730)	1:22:A:TRP:HH2	1:26:A:LYS:HB2	8	0.18
(1,690)	1:4:A:PHE:HB2	1:5:A:VAL:H	6	0.18
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG21	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG22	8	0.18
(1,616)	1:143:A:GLN:HE22	1:177:A:THR:HG23	8	0.18
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	6	0.18
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG21	6	0.18
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG22	6	0.18
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG23	6	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	1	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	1	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	1	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	2	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	2	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	2	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	4	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	4	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	4	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	5	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	5	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	5	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	6	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	6	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	6	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	7	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	7	0.18
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	7	0.18
(1,263)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	7	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG11	3	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG12	3	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG13	3	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG21	3	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG22	3	0.18
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG23	3	0.18
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	9	0.18
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	9	0.18
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	9	0.18
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	9	0.18
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	9	0.18
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	9	0.18
(1,219)	1:56:A:SER:H	1:53:A:ALA:HB1	10	0.18
(1,219)	1:56:A:SER:H	1:53:A:ALA:HB2	10	0.18
(1,219)	1:56:A:SER:H	1:53:A:ALA:HB3	10	0.18
(1,167)	1:174:A:CYS:H	1:170:A:ARG:HA	1	0.18
(1,90)	1:27:A:LYS:HE2	1:27:A:LYS:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:27:A:LYS:HE3	1:27:A:LYS:H	5	0.18
(1,3584)	1:168:A:GLN:H	1:180:A:LEU:H	10	0.17
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD11	1	0.17
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD12	1	0.17
(1,3392)	1:59:A:LEU:HD11	1:61:A:LEU:HD13	1	0.17
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD11	1	0.17
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD12	1	0.17
(1,3392)	1:59:A:LEU:HD12	1:61:A:LEU:HD13	1	0.17
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD11	1	0.17
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD12	1	0.17
(1,3392)	1:59:A:LEU:HD13	1:61:A:LEU:HD13	1	0.17
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD11	2	0.17
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD12	2	0.17
(1,3320)	1:61:A:LEU:HA	1:61:A:LEU:HD13	2	0.17
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD1	6	0.17
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD2	6	0.17
(1,3183)	1:175:A:ASP:H	1:174:A:CYS:HB2	3	0.17
(1,2930)	1:61:A:LEU:HD11	1:66:A:ILE:H	1	0.17
(1,2930)	1:61:A:LEU:HD12	1:66:A:ILE:H	1	0.17
(1,2930)	1:61:A:LEU:HD13	1:66:A:ILE:H	1	0.17
(1,2930)	1:61:A:LEU:HD11	1:66:A:ILE:H	8	0.17
(1,2930)	1:61:A:LEU:HD12	1:66:A:ILE:H	8	0.17
(1,2930)	1:61:A:LEU:HD13	1:66:A:ILE:H	8	0.17
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	5	0.17
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD11	1	0.17
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD12	1	0.17
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD13	1	0.17
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD21	1	0.17
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD22	1	0.17
(1,2774)	1:131:A:LEU:HB2	1:131:A:LEU:HD23	1	0.17
(1,2680)	1:180:A:LEU:HA	1:167:A:ILE:H	4	0.17
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	5	0.17
(1,2675)	1:60:A:ASN:HD22	1:60:A:ASN:HB2	1	0.17
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	8	0.17
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	8	0.17
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	8	0.17
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	10	0.17
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	10	0.17
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	10	0.17
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	10	0.17
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	10	0.17
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB1	8	0.17
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB2	8	0.17
(1,2320)	1:30:A:GLN:H	1:54:A:ALA:HB3	8	0.17
(1,2296)	1:37:A:PHE:HA	1:38:A:LEU:H	3	0.17
(1,2253)	1:94:A:VAL:HB	1:160:A:THR:H	6	0.17
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD11	4	0.17
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD12	4	0.17
(1,2229)	1:48:A:THR:HA	1:51:A:LEU:HD13	4	0.17
(1,2226)	1:161:A:GLU:HG3	1:161:A:GLU:H	5	0.17
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	5	0.17
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	7	0.17
(1,2136)	1:155:A:GLN:HG2	1:157:A:ILE:H	2	0.17
(1,2130)	1:167:A:ILE:HG12	1:179:A:PHE:H	3	0.17
(1,2118)	1:94:A:VAL:HG21	1:96:A:GLU:H	8	0.17
(1,2118)	1:94:A:VAL:HG22	1:96:A:GLU:H	8	0.17
(1,2118)	1:94:A:VAL:HG23	1:96:A:GLU:H	8	0.17
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG21	8	0.17
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG22	8	0.17
(1,2045)	1:59:A:LEU:HA	1:21:A:VAL:HG23	8	0.17
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD11	4	0.17
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD12	4	0.17
(1,1994)	1:14:A:ILE:HB	1:14:A:ILE:HD13	4	0.17
(1,1990)	1:26:A:LYS:HE3	1:35:A:GLY:H	1	0.17
(1,1901)	1:131:A:LEU:HG	1:131:A:LEU:H	4	0.17
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD11	5	0.17
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD12	5	0.17
(1,1816)	1:69:A:MET:HE1	1:59:A:LEU:HD13	5	0.17
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD11	5	0.17
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD12	5	0.17
(1,1816)	1:69:A:MET:HE2	1:59:A:LEU:HD13	5	0.17
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD11	5	0.17
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD12	5	0.17
(1,1816)	1:69:A:MET:HE3	1:59:A:LEU:HD13	5	0.17
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	9	0.17
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	9	0.17
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	9	0.17
(1,1600)	1:184:A:LYS:HA	1:160:A:THR:HG21	4	0.17
(1,1600)	1:184:A:LYS:HA	1:160:A:THR:HG22	4	0.17
(1,1600)	1:184:A:LYS:HA	1:160:A:THR:HG23	4	0.17
(1,1530)	1:126:A:GLU:HG3	1:127:A:LYS:H	8	0.17
(1,1481)	1:112:A:TYR:HE1	1:111:A:ILE:HD11	10	0.17
(1,1481)	1:112:A:TYR:HE1	1:111:A:ILE:HD12	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1481)	1:112:A:TYR:HE1	1:111:A:ILE:HD13	10	0.17
(1,1481)	1:112:A:TYR:HE2	1:111:A:ILE:HD11	10	0.17
(1,1481)	1:112:A:TYR:HE2	1:111:A:ILE:HD12	10	0.17
(1,1481)	1:112:A:TYR:HE2	1:111:A:ILE:HD13	10	0.17
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	9	0.17
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	9	0.17
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	9	0.17
(1,1439)	1:99:A:GLN:HE22	1:95:A:ARG:HG2	2	0.17
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	5	0.17
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	5	0.17
(1,1409)	1:14:A:ILE:HB	1:18:A:GLY:H	9	0.17
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG11	8	0.17
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG12	8	0.17
(1,1383)	1:59:A:LEU:HD21	1:21:A:VAL:HG13	8	0.17
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG11	8	0.17
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG12	8	0.17
(1,1383)	1:59:A:LEU:HD22	1:21:A:VAL:HG13	8	0.17
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG11	8	0.17
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG12	8	0.17
(1,1383)	1:59:A:LEU:HD23	1:21:A:VAL:HG13	8	0.17
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	1	0.17
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	1	0.17
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	1	0.17
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	6	0.17
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	6	0.17
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	6	0.17
(1,1345)	1:19:A:PRO:HD2	1:18:A:GLY:H	10	0.17
(1,1246)	1:158:A:HIS:HD2	1:159:A:GLY:H	1	0.17
(1,1138)	1:73:A:MET:HE1	1:16:A:ASN:H	9	0.17
(1,1138)	1:73:A:MET:HE2	1:16:A:ASN:H	9	0.17
(1,1138)	1:73:A:MET:HE3	1:16:A:ASN:H	9	0.17
(1,1053)	1:162:A:ILE:HA	1:164:A:MET:H	7	0.17
(1,1053)	1:162:A:ILE:HA	1:164:A:MET:H	10	0.17
(1,1035)	1:170:A:ARG:HE	1:170:A:ARG:HG3	4	0.17
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG21	10	0.17
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG22	10	0.17
(1,999)	1:158:A:HIS:H	1:94:A:VAL:HG23	10	0.17
(1,935)	1:125:A:ALA:HA	1:132:A:ILE:HB	1	0.17
(1,853)	1:171:A:ASN:HD22	1:173:A:GLU:H	7	0.17
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD21	9	0.17
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD22	9	0.17
(1,745)	1:32:A:ASP:H	1:51:A:LEU:HD23	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,732)	1:157:A:ILE:HB	1:158:A:HIS:H	5	0.17
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	4	0.17
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	4	0.17
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	4	0.17
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG11	9	0.17
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG12	9	0.17
(1,659)	1:143:A:GLN:H	1:166:A:VAL:HG13	9	0.17
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	5	0.17
(1,524)	1:124:A:ASP:HB2	1:131:A:LEU:H	4	0.17
(1,500)	1:23:A:GLU:HB3	1:25:A:ILE:H	9	0.17
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG21	9	0.17
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG22	9	0.17
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG23	9	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	3	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	3	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	3	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	8	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	8	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	8	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	9	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	9	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	9	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG11	10	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG12	10	0.17
(1,382)	1:39:A:VAL:HB	1:39:A:VAL:HG13	10	0.17
(1,381)	1:100:A:ASN:H	1:99:A:GLN:H	4	0.17
(1,271)	1:150:A:ILE:HD11	2:201:A:Z90:HAI	5	0.17
(1,271)	1:150:A:ILE:HD12	2:201:A:Z90:HAI	5	0.17
(1,271)	1:150:A:ILE:HD13	2:201:A:Z90:HAI	5	0.17
(1,268)	1:101:A:LEU:HD21	2:201:A:Z90:HAI	6	0.17
(1,268)	1:101:A:LEU:HD22	2:201:A:Z90:HAI	6	0.17
(1,268)	1:101:A:LEU:HD23	2:201:A:Z90:HAI	6	0.17
(1,261)	2:201:A:Z90:HAI	2:201:A:Z90:HBD	5	0.17
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG21	4	0.17
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG22	4	0.17
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG23	4	0.17
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB1	8	0.17
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB2	8	0.17
(1,233)	1:159:A:GLY:H	1:154:A:ALA:HB3	8	0.17
(1,69)	1:142:A:LEU:HD11	1:67:A:LEU:HD21	6	0.17
(1,69)	1:142:A:LEU:HD11	1:67:A:LEU:HD22	6	0.17
(1,69)	1:142:A:LEU:HD11	1:67:A:LEU:HD23	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:142:A:LEU:HD12	1:67:A:LEU:HD21	6	0.17
(1,69)	1:142:A:LEU:HD12	1:67:A:LEU:HD22	6	0.17
(1,69)	1:142:A:LEU:HD12	1:67:A:LEU:HD23	6	0.17
(1,69)	1:142:A:LEU:HD13	1:67:A:LEU:HD21	6	0.17
(1,69)	1:142:A:LEU:HD13	1:67:A:LEU:HD22	6	0.17
(1,69)	1:142:A:LEU:HD13	1:67:A:LEU:HD23	6	0.17
(1,3540)	1:54:A:ALA:HB1	1:28:A:GLU:H	2	0.16
(1,3540)	1:54:A:ALA:HB2	1:28:A:GLU:H	2	0.16
(1,3540)	1:54:A:ALA:HB3	1:28:A:GLU:H	2	0.16
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG21	8	0.16
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG22	8	0.16
(1,3522)	1:143:A:GLN:HE22	1:177:A:THR:HG23	8	0.16
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD11	7	0.16
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD12	7	0.16
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD13	7	0.16
(1,3455)	1:95:A:ARG:HD2	1:96:A:GLU:H	2	0.16
(1,3455)	1:95:A:ARG:HD3	1:96:A:GLU:H	2	0.16
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	8	0.16
(1,3366)	1:125:A:ALA:HA	1:132:A:ILE:HD11	10	0.16
(1,3366)	1:125:A:ALA:HA	1:132:A:ILE:HD12	10	0.16
(1,3366)	1:125:A:ALA:HA	1:132:A:ILE:HD13	10	0.16
(1,3353)	1:91:A:GLY:H	1:93:A:ASN:H	10	0.16
(1,3344)	1:59:A:LEU:HA	1:59:A:LEU:HD11	2	0.16
(1,3344)	1:59:A:LEU:HA	1:59:A:LEU:HD12	2	0.16
(1,3344)	1:59:A:LEU:HA	1:59:A:LEU:HD13	2	0.16
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD11	4	0.16
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD12	4	0.16
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD13	4	0.16
(1,3284)	1:100:A:ASN:HB3	1:103:A:ALA:H	5	0.16
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD11	4	0.16
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD12	4	0.16
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD13	4	0.16
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	3	0.16
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	5	0.16
(1,3207)	1:35:A:GLY:HA3	1:36:A:GLN:H	2	0.16
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	10	0.16
(1,3041)	1:146:A:VAL:HG11	1:146:A:VAL:HA	9	0.16
(1,3041)	1:146:A:VAL:HG12	1:146:A:VAL:HA	9	0.16
(1,3041)	1:146:A:VAL:HG13	1:146:A:VAL:HA	9	0.16
(1,3041)	1:146:A:VAL:HG21	1:146:A:VAL:HA	9	0.16
(1,3041)	1:146:A:VAL:HG22	1:146:A:VAL:HA	9	0.16
(1,3041)	1:146:A:VAL:HG23	1:146:A:VAL:HA	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD11	9	0.16
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD12	9	0.16
(1,3029)	1:101:A:LEU:HD21	1:98:A:LEU:HD13	9	0.16
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD11	9	0.16
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD12	9	0.16
(1,3029)	1:101:A:LEU:HD22	1:98:A:LEU:HD13	9	0.16
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD11	9	0.16
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD12	9	0.16
(1,3029)	1:101:A:LEU:HD23	1:98:A:LEU:HD13	9	0.16
(1,3001)	1:137:A:SER:H	1:136:A:TYR:HB2	9	0.16
(1,2961)	1:123:A:THR:HB	1:124:A:ASP:H	7	0.16
(1,2795)	1:16:A:ASN:HD22	1:16:A:ASN:H	2	0.16
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	10	0.16
(1,2676)	1:153:A:VAL:HG21	1:153:A:VAL:H	1	0.16
(1,2676)	1:153:A:VAL:HG22	1:153:A:VAL:H	1	0.16
(1,2676)	1:153:A:VAL:HG23	1:153:A:VAL:H	1	0.16
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	5	0.16
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG21	4	0.16
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG22	4	0.16
(1,2637)	1:125:A:ALA:H	1:132:A:ILE:HG23	4	0.16
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG11	6	0.16
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG12	6	0.16
(1,2608)	1:48:A:THR:HG21	1:52:A:VAL:HG13	6	0.16
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG11	6	0.16
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG12	6	0.16
(1,2608)	1:48:A:THR:HG22	1:52:A:VAL:HG13	6	0.16
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG11	6	0.16
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG12	6	0.16
(1,2608)	1:48:A:THR:HG23	1:52:A:VAL:HG13	6	0.16
(1,2466)	1:95:A:ARG:H	1:93:A:ASN:H	10	0.16
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD11	5	0.16
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD12	5	0.16
(1,2459)	1:141:A:GLY:H	1:142:A:LEU:HD13	5	0.16
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG21	3	0.16
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG22	3	0.16
(1,2457)	1:166:A:VAL:H	1:166:A:VAL:HG23	3	0.16
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	1	0.16
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	1	0.16
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	1	0.16
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	1	0.16
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	1	0.16
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2415)	1:75:A:PHE:HE1	1:156:A:GLN:H	8	0.16
(1,2415)	1:75:A:PHE:HE2	1:156:A:GLN:H	8	0.16
(1,2242)	1:173:A:GLU:HG2	1:174:A:CYS:H	4	0.16
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD11	1	0.16
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD12	1	0.16
(1,2239)	1:22:A:TRP:HH2	1:51:A:LEU:HD13	1	0.16
(1,2177)	1:186:A:SER:H	1:160:A:THR:HA	9	0.16
(1,2163)	1:69:A:MET:HE1	1:66:A:ILE:H	6	0.16
(1,2163)	1:69:A:MET:HE2	1:66:A:ILE:H	6	0.16
(1,2163)	1:69:A:MET:HE3	1:66:A:ILE:H	6	0.16
(1,2155)	1:125:A:ALA:HA	1:126:A:GLU:H	2	0.16
(1,1966)	1:81:A:SER:H	1:80:A:GLU:H	5	0.16
(1,1949)	1:175:A:ASP:H	1:170:A:ARG:HG3	8	0.16
(1,1901)	1:131:A:LEU:HG	1:131:A:LEU:H	8	0.16
(1,1876)	1:10:A:GLU:HG3	1:22:A:TRP:HE1	7	0.16
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD21	5	0.16
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD22	5	0.16
(1,1866)	1:134:A:HIS:H	1:133:A:LEU:HD23	5	0.16
(1,1864)	1:38:A:LEU:HB2	1:41:A:ILE:H	7	0.16
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	2	0.16
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	2	0.16
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	5	0.16
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	5	0.16
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	6	0.16
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	6	0.16
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	10	0.16
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	10	0.16
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD11	3	0.16
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD12	3	0.16
(1,1632)	1:149:A:ILE:HB	1:149:A:ILE:HD13	3	0.16
(1,1595)	1:164:A:MET:HE1	1:147:A:ILE:HD11	10	0.16
(1,1595)	1:164:A:MET:HE1	1:147:A:ILE:HD12	10	0.16
(1,1595)	1:164:A:MET:HE1	1:147:A:ILE:HD13	10	0.16
(1,1595)	1:164:A:MET:HE2	1:147:A:ILE:HD11	10	0.16
(1,1595)	1:164:A:MET:HE2	1:147:A:ILE:HD12	10	0.16
(1,1595)	1:164:A:MET:HE2	1:147:A:ILE:HD13	10	0.16
(1,1595)	1:164:A:MET:HE3	1:147:A:ILE:HD11	10	0.16
(1,1595)	1:164:A:MET:HE3	1:147:A:ILE:HD12	10	0.16
(1,1595)	1:164:A:MET:HE3	1:147:A:ILE:HD13	10	0.16
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG21	7	0.16
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG22	7	0.16
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG23	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1567)	1:29:A:ALA:HA	1:54:A:ALA:H	9	0.16
(1,1565)	1:171:A:ASN:HD22	1:169:A:GLN:HE22	5	0.16
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD21	2	0.16
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD22	2	0.16
(1,1527)	1:145:A:ILE:HG12	1:142:A:LEU:HD23	2	0.16
(1,1502)	1:57:A:LYS:HG2	1:58:A:VAL:H	6	0.16
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD21	8	0.16
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD22	8	0.16
(1,1261)	1:150:A:ILE:HD11	1:98:A:LEU:HD23	8	0.16
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD21	8	0.16
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD22	8	0.16
(1,1261)	1:150:A:ILE:HD12	1:98:A:LEU:HD23	8	0.16
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD21	8	0.16
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD22	8	0.16
(1,1261)	1:150:A:ILE:HD13	1:98:A:LEU:HD23	8	0.16
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG21	3	0.16
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG22	3	0.16
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG23	3	0.16
(1,1169)	1:17:A:TYR:HE1	1:16:A:ASN:H	5	0.16
(1,1169)	1:17:A:TYR:HE2	1:16:A:ASN:H	5	0.16
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	1	0.16
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	1	0.16
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	1	0.16
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG21	5	0.16
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG22	5	0.16
(1,1105)	1:157:A:ILE:H	1:153:A:VAL:HG23	5	0.16
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	4	0.16
(1,1018)	1:170:A:ARG:HD2	1:169:A:GLN:H	9	0.16
(1,1018)	1:170:A:ARG:HD3	1:169:A:GLN:H	9	0.16
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	1	0.16
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	8	0.16
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD11	4	0.16
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD12	4	0.16
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD13	4	0.16
(1,912)	1:71:A:GLY:H	1:67:A:LEU:H	5	0.16
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD11	8	0.16
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD12	8	0.16
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD13	8	0.16
(1,778)	1:120:A:PHE:H	1:101:A:LEU:HB2	2	0.16
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	10	0.16
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	10	0.16
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:127:A:LYS:HA	1:128:A:GLY:HA3	3	0.16
(1,677)	1:120:A:PHE:H	1:136:A:TYR:HB2	3	0.16
(1,656)	1:169:A:GLN:HA	1:166:A:VAL:HG21	3	0.16
(1,656)	1:169:A:GLN:HA	1:166:A:VAL:HG22	3	0.16
(1,656)	1:169:A:GLN:HA	1:166:A:VAL:HG23	3	0.16
(1,598)	1:143:A:GLN:HA	1:143:A:GLN:HE22	2	0.16
(1,579)	1:173:A:GLU:HB2	1:171:A:ASN:H	3	0.16
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	5	0.16
(1,444)	1:131:A:LEU:HG	1:132:A:ILE:H	10	0.16
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG21	1	0.16
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG22	1	0.16
(1,403)	1:183:A:GLU:HG3	1:160:A:THR:HG23	1	0.16
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	6	0.16
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	6	0.16
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	6	0.16
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	6	0.16
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	6	0.16
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	6	0.16
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	4	0.16
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	4	0.16
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	9	0.16
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	9	0.16
(1,161)	1:176:A:HIS:H	1:171:A:ASN:H	3	0.16
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	8	0.16
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	8	0.16
(1,3565)	1:131:A:LEU:HG	1:181:A:ILE:H	1	0.15
(1,3549)	1:165:A:LYS:HG2	1:180:A:LEU:H	10	0.15
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	2	0.15
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	3	0.15
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	4	0.15
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	10	0.15
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	5	0.15
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	5	0.15
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	5	0.15
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	5	0.15
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	5	0.15
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	5	0.15
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	5	0.15
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	5	0.15
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	5	0.15
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD21	3	0.15
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD22	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3394)	1:59:A:LEU:HA	1:61:A:LEU:HD23	3	0.15
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE1	7	0.15
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE2	7	0.15
(1,3378)	1:66:A:ILE:HA	1:69:A:MET:HE3	7	0.15
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD11	8	0.15
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD12	8	0.15
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD13	8	0.15
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD11	10	0.15
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD12	10	0.15
(1,3333)	1:132:A:ILE:HA	1:132:A:ILE:HD13	10	0.15
(1,3297)	1:143:A:GLN:HE22	1:142:A:LEU:H	8	0.15
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG11	4	0.15
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG12	4	0.15
(1,3294)	1:59:A:LEU:HA	1:21:A:VAL:HG13	4	0.15
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG21	2	0.15
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG22	2	0.15
(1,3291)	1:154:A:ALA:HA	1:160:A:THR:HG23	2	0.15
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD11	3	0.15
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD12	3	0.15
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD13	3	0.15
(1,3220)	1:27:A:LYS:HG3	1:27:A:LYS:H	4	0.15
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	1	0.15
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	2	0.15
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	6	0.15
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	8	0.15
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	10	0.15
(1,3207)	1:35:A:GLY:HA3	1:36:A:GLN:H	7	0.15
(1,3197)	1:139:A:ARG:HG2	1:140:A:GLU:H	1	0.15
(1,3137)	1:19:A:PRO:HD3	1:22:A:TRP:H	9	0.15
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	4	0.15
(1,3044)	1:136:A:TYR:HD1	1:119:A:SER:H	9	0.15
(1,3044)	1:136:A:TYR:HD2	1:119:A:SER:H	9	0.15
(1,2966)	1:138:A:GLU:HG2	1:138:A:GLU:H	6	0.15
(1,2966)	1:138:A:GLU:HG3	1:138:A:GLU:H	6	0.15
(1,2863)	1:126:A:GLU:H	1:130:A:GLY:H	9	0.15
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD1	9	0.15
(1,2829)	1:5:A:VAL:HA	1:2:A:TYR:HD2	9	0.15
(1,2734)	1:14:A:ILE:HB	1:16:A:ASN:H	9	0.15
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	3	0.15
(1,2658)	1:55:A:ALA:HA	1:61:A:LEU:H	2	0.15
(1,2560)	1:141:A:GLY:HA3	1:144:A:ASP:H	3	0.15
(1,2439)	1:112:A:TYR:HD1	1:108:A:LEU:HD11	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2439)	1:112:A:TYR:HD1	1:108:A:LEU:HD12	2	0.15
(1,2439)	1:112:A:TYR:HD1	1:108:A:LEU:HD13	2	0.15
(1,2439)	1:112:A:TYR:HD1	1:108:A:LEU:HD21	2	0.15
(1,2439)	1:112:A:TYR:HD1	1:108:A:LEU:HD22	2	0.15
(1,2439)	1:112:A:TYR:HD1	1:108:A:LEU:HD23	2	0.15
(1,2439)	1:112:A:TYR:HD2	1:108:A:LEU:HD11	2	0.15
(1,2439)	1:112:A:TYR:HD2	1:108:A:LEU:HD12	2	0.15
(1,2439)	1:112:A:TYR:HD2	1:108:A:LEU:HD13	2	0.15
(1,2439)	1:112:A:TYR:HD2	1:108:A:LEU:HD21	2	0.15
(1,2439)	1:112:A:TYR:HD2	1:108:A:LEU:HD22	2	0.15
(1,2439)	1:112:A:TYR:HD2	1:108:A:LEU:HD23	2	0.15
(1,2438)	1:104:A:LEU:HD21	1:90:A:LEU:HD21	1	0.15
(1,2438)	1:104:A:LEU:HD21	1:90:A:LEU:HD22	1	0.15
(1,2438)	1:104:A:LEU:HD21	1:90:A:LEU:HD23	1	0.15
(1,2438)	1:104:A:LEU:HD22	1:90:A:LEU:HD21	1	0.15
(1,2438)	1:104:A:LEU:HD22	1:90:A:LEU:HD22	1	0.15
(1,2438)	1:104:A:LEU:HD22	1:90:A:LEU:HD23	1	0.15
(1,2438)	1:104:A:LEU:HD23	1:90:A:LEU:HD21	1	0.15
(1,2438)	1:104:A:LEU:HD23	1:90:A:LEU:HD22	1	0.15
(1,2438)	1:104:A:LEU:HD23	1:90:A:LEU:HD23	1	0.15
(1,2423)	1:183:A:GLU:HB3	1:184:A:LYS:H	10	0.15
(1,2183)	1:120:A:PHE:HA	1:121:A:ARG:H	6	0.15
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD11	8	0.15
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD12	8	0.15
(1,2096)	1:132:A:ILE:HG12	1:167:A:ILE:HD13	8	0.15
(1,1935)	1:135:A:TYR:HD1	1:119:A:SER:H	8	0.15
(1,1935)	1:135:A:TYR:HD2	1:119:A:SER:H	8	0.15
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	1	0.15
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	1	0.15
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	4	0.15
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	4	0.15
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	7	0.15
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	7	0.15
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	9	0.15
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	9	0.15
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD2	5	0.15
(1,1840)	1:170:A:ARG:HE	1:170:A:ARG:HD3	5	0.15
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB1	6	0.15
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB2	6	0.15
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB3	6	0.15
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	4	0.15
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	4	0.15
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG21	1	0.15
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG22	1	0.15
(1,1354)	1:150:A:ILE:HA	1:153:A:VAL:HG23	1	0.15
(1,1247)	1:165:A:LYS:HA	1:147:A:ILE:HD11	10	0.15
(1,1247)	1:165:A:LYS:HA	1:147:A:ILE:HD12	10	0.15
(1,1247)	1:165:A:LYS:HA	1:147:A:ILE:HD13	10	0.15
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	2	0.15
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	2	0.15
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	2	0.15
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	2	0.15
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	2	0.15
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	2	0.15
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	2	0.15
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	2	0.15
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	2	0.15
(1,1169)	1:17:A:TYR:HE1	1:16:A:ASN:H	7	0.15
(1,1169)	1:17:A:TYR:HE2	1:16:A:ASN:H	7	0.15
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	2	0.15
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	4	0.15
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	10	0.15
(1,867)	1:165:A:LYS:HD2	1:165:A:LYS:H	7	0.15
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD11	7	0.15
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD12	7	0.15
(1,854)	1:41:A:ILE:HA	1:42:A:ILE:HD13	7	0.15
(1,818)	1:114:A:GLY:H	1:115:A:MET:H	9	0.15
(1,681)	1:177:A:THR:HB	1:135:A:TYR:H	2	0.15
(1,617)	1:3:A:GLY:H	1:43:A:TYR:H	7	0.15
(1,535)	1:129:A:LYS:HA	1:131:A:LEU:H	2	0.15
(1,531)	1:124:A:ASP:HA	1:131:A:LEU:H	2	0.15
(1,487)	1:124:A:ASP:HB2	1:132:A:ILE:H	2	0.15
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	6	0.15
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG21	3	0.15
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG22	3	0.15
(1,421)	1:158:A:HIS:HD2	1:157:A:ILE:HG23	3	0.15
(1,420)	1:136:A:TYR:HB3	1:119:A:SER:H	6	0.15
(1,381)	1:100:A:ASN:H	1:99:A:GLN:H	1	0.15
(1,298)	2:201:A:Z90:HAM	2:201:A:Z90:HBD	1	0.15
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	4	0.15
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	4	0.15
(1,232)	1:155:A:GLN:H	1:162:A:ILE:HD11	10	0.15
(1,232)	1:155:A:GLN:H	1:162:A:ILE:HD12	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,232)	1:155:A:GLN:H	1:162:A:ILE:HD13	10	0.15
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG11	8	0.15
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG12	8	0.15
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG13	8	0.15
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG21	8	0.15
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG22	8	0.15
(1,226)	1:63:A:ALA:H	1:52:A:VAL:HG23	8	0.15
(1,158)	1:161:A:GLU:H	1:160:A:THR:H	4	0.15
(1,114)	1:182:A:GLU:H	1:164:A:MET:H	7	0.15
(1,99)	1:125:A:ALA:HA	1:132:A:ILE:H	10	0.15
(1,96)	1:180:A:LEU:HG	1:131:A:LEU:H	4	0.15
(1,9)	1:127:A:LYS:HA	1:128:A:GLY:HA2	3	0.15
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD11	5	0.14
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD12	5	0.14
(1,3472)	1:125:A:ALA:H	1:132:A:ILE:HD13	5	0.14
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD11	9	0.14
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD12	9	0.14
(1,3454)	1:101:A:LEU:HD11	1:98:A:LEU:HD13	9	0.14
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD11	9	0.14
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD12	9	0.14
(1,3454)	1:101:A:LEU:HD12	1:98:A:LEU:HD13	9	0.14
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD11	9	0.14
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD12	9	0.14
(1,3454)	1:101:A:LEU:HD13	1:98:A:LEU:HD13	9	0.14
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	1	0.14
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	5	0.14
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	6	0.14
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	7	0.14
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	8	0.14
(1,3433)	1:163:A:ASP:HB2	1:163:A:ASP:HB3	9	0.14
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD11	6	0.14
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD12	6	0.14
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD13	6	0.14
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	4	0.14
(1,3210)	1:3:A:GLY:H	1:3:A:GLY:HA3	9	0.14
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	5	0.14
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	5	0.14
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	5	0.14
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	6	0.14
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	6	0.14
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	6	0.14
(1,2995)	1:176:A:HIS:HA	1:137:A:SER:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2908)	1:58:A:VAL:H	1:59:A:LEU:HD21	2	0.14
(1,2908)	1:58:A:VAL:H	1:59:A:LEU:HD22	2	0.14
(1,2908)	1:58:A:VAL:H	1:59:A:LEU:HD23	2	0.14
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	1	0.14
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	8	0.14
(1,2786)	1:14:A:ILE:HG13	1:22:A:TRP:HE1	6	0.14
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	1	0.14
(1,2680)	1:180:A:LEU:HA	1:167:A:ILE:H	10	0.14
(1,2676)	1:153:A:VAL:HG21	1:153:A:VAL:H	6	0.14
(1,2676)	1:153:A:VAL:HG22	1:153:A:VAL:H	6	0.14
(1,2676)	1:153:A:VAL:HG23	1:153:A:VAL:H	6	0.14
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG21	10	0.14
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG22	10	0.14
(1,2550)	1:183:A:GLU:HG2	1:162:A:ILE:HG23	10	0.14
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	9	0.14
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	9	0.14
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	9	0.14
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB1	9	0.14
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB2	9	0.14
(1,2529)	1:25:A:ILE:HA	1:54:A:ALA:HB3	9	0.14
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD11	10	0.14
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD12	10	0.14
(1,2494)	1:51:A:LEU:H	1:31:A:LEU:HD13	10	0.14
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD21	2	0.14
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD22	2	0.14
(1,2448)	1:51:A:LEU:H	1:9:A:LEU:HD23	2	0.14
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	9	0.14
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	9	0.14
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	9	0.14
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	9	0.14
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	9	0.14
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	9	0.14
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG21	9	0.14
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG22	9	0.14
(1,2354)	1:110:A:THR:HA	1:110:A:THR:HG23	9	0.14
(1,2280)	1:65:A:GLU:HA	1:64:A:GLY:H	6	0.14
(1,2247)	1:174:A:CYS:H	1:174:A:CYS:HB3	3	0.14
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB1	2	0.14
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB2	2	0.14
(1,2231)	1:129:A:LYS:HA	1:125:A:ALA:HB3	2	0.14
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG21	6	0.14
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG22	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2152)	1:144:A:ASP:H	1:166:A:VAL:HG23	6	0.14
(1,2005)	1:47:A:LYS:HE3	1:47:A:LYS:H	3	0.14
(1,1988)	1:26:A:LYS:HB3	1:23:A:GLU:H	2	0.14
(1,1854)	1:9:A:LEU:HB2	1:9:A:LEU:H	8	0.14
(1,1854)	1:9:A:LEU:HB3	1:9:A:LEU:H	8	0.14
(1,1843)	1:62:A:ASN:HD22	1:65:A:GLU:H	10	0.14
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE1	1	0.14
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE2	1	0.14
(1,1798)	1:66:A:ILE:HG13	1:69:A:MET:HE3	1	0.14
(1,1672)	1:173:A:GLU:HG3	1:174:A:CYS:H	3	0.14
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG21	3	0.14
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG22	3	0.14
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG23	3	0.14
(1,1497)	1:80:A:GLU:HB2	1:82:A:GLY:H	5	0.14
(1,1497)	1:80:A:GLU:HB2	1:82:A:GLY:H	6	0.14
(1,1301)	1:176:A:HIS:HA	1:170:A:ARG:H	9	0.14
(1,1297)	1:145:A:ILE:HG12	1:71:A:GLY:H	8	0.14
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	9	0.14
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	9	0.14
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	9	0.14
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	9	0.14
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	9	0.14
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	9	0.14
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	9	0.14
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	9	0.14
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	9	0.14
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD11	8	0.14
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD12	8	0.14
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD13	8	0.14
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD11	7	0.14
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD12	7	0.14
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD13	7	0.14
(1,1169)	1:17:A:TYR:HE1	1:16:A:ASN:H	3	0.14
(1,1169)	1:17:A:TYR:HE2	1:16:A:ASN:H	3	0.14
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	3	0.14
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	3	0.14
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	3	0.14
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD21	8	0.14
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD22	8	0.14
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD23	8	0.14
(1,1067)	1:144:A:ASP:H	1:67:A:LEU:HD21	5	0.14
(1,1067)	1:144:A:ASP:H	1:67:A:LEU:HD22	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:144:A:ASP:H	1:67:A:LEU:HD23	5	0.14
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	3	0.14
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	3	0.14
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	3	0.14
(1,986)	1:22:A:TRP:HD1	1:26:A:LYS:H	5	0.14
(1,948)	1:50:A:ASP:HB2	1:53:A:ALA:H	10	0.14
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	6	0.14
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	9	0.14
(1,922)	1:69:A:MET:HG3	1:69:A:MET:H	7	0.14
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	6	0.14
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	6	0.14
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	6	0.14
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	8	0.14
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	8	0.14
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	8	0.14
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	1	0.14
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	1	0.14
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	1	0.14
(1,649)	1:33:A:GLU:H	1:31:A:LEU:H	7	0.14
(1,501)	1:126:A:GLU:HG3	1:126:A:GLU:H	9	0.14
(1,466)	1:15:A:ARG:HA	1:17:A:TYR:H	2	0.14
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	4	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	1	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	1	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	1	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	2	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	2	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	2	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	10	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	10	0.14
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	10	0.14
(1,317)	1:101:A:LEU:HD11	2:201:A:Z90:HAI	5	0.14
(1,317)	1:101:A:LEU:HD12	2:201:A:Z90:HAI	5	0.14
(1,317)	1:101:A:LEU:HD13	2:201:A:Z90:HAI	5	0.14
(1,317)	1:101:A:LEU:HD11	2:201:A:Z90:HAI	9	0.14
(1,317)	1:101:A:LEU:HD12	2:201:A:Z90:HAI	9	0.14
(1,317)	1:101:A:LEU:HD13	2:201:A:Z90:HAI	9	0.14
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	7	0.14
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	7	0.14
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG21	5	0.14
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG22	5	0.14
(1,240)	1:69:A:MET:H	1:66:A:ILE:HG23	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB1	6	0.14
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB2	6	0.14
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB3	6	0.14
(1,181)	1:40:A:ARG:HG2	1:40:A:ARG:H	4	0.14
(1,181)	1:40:A:ARG:HG3	1:40:A:ARG:H	4	0.14
(1,105)	1:165:A:LYS:H	1:182:A:GLU:H	2	0.14
(1,90)	1:27:A:LYS:HE2	1:27:A:LYS:H	4	0.14
(1,90)	1:27:A:LYS:HE3	1:27:A:LYS:H	4	0.14
(1,88)	1:27:A:LYS:HB2	1:26:A:LYS:H	10	0.14
(1,88)	1:27:A:LYS:HB3	1:26:A:LYS:H	10	0.14
(1,87)	1:27:A:LYS:HB2	1:24:A:ASP:H	8	0.14
(1,87)	1:27:A:LYS:HB3	1:24:A:ASP:H	8	0.14
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG21	2	0.13
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG22	2	0.13
(1,3533)	1:22:A:TRP:HD1	1:14:A:ILE:HG23	2	0.13
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD21	5	0.13
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD22	5	0.13
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD23	5	0.13
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD21	5	0.13
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD22	5	0.13
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD23	5	0.13
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD21	5	0.13
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD22	5	0.13
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD23	5	0.13
(1,3402)	1:49:A:TYR:HA	1:48:A:THR:H	9	0.13
(1,3354)	1:27:A:LYS:HD3	1:28:A:GLU:H	7	0.13
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD1	9	0.13
(1,3264)	1:3:A:GLY:HA2	1:43:A:TYR:HD2	9	0.13
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD11	10	0.13
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD12	10	0.13
(1,3263)	1:154:A:ALA:HA	1:157:A:ILE:HD13	10	0.13
(1,3262)	1:46:A:SER:H	1:44:A:ASP:HB2	6	0.13
(1,3207)	1:35:A:GLY:HA3	1:36:A:GLN:H	5	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	1	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	1	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	1	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	2	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	2	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	2	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	3	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	3	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	4	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	4	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	4	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	8	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	8	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	8	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	10	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	10	0.13
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	10	0.13
(1,3099)	1:8:A:ALA:HB1	1:12:A:LEU:H	2	0.13
(1,3099)	1:8:A:ALA:HB2	1:12:A:LEU:H	2	0.13
(1,3099)	1:8:A:ALA:HB3	1:12:A:LEU:H	2	0.13
(1,3097)	1:78:A:CYS:HB3	1:77:A:PHE:H	10	0.13
(1,3056)	1:3:A:GLY:H	1:3:A:GLY:HA2	7	0.13
(1,3004)	1:69:A:MET:HE1	1:61:A:LEU:HD21	7	0.13
(1,3004)	1:69:A:MET:HE1	1:61:A:LEU:HD22	7	0.13
(1,3004)	1:69:A:MET:HE1	1:61:A:LEU:HD23	7	0.13
(1,3004)	1:69:A:MET:HE2	1:61:A:LEU:HD21	7	0.13
(1,3004)	1:69:A:MET:HE2	1:61:A:LEU:HD22	7	0.13
(1,3004)	1:69:A:MET:HE2	1:61:A:LEU:HD23	7	0.13
(1,3004)	1:69:A:MET:HE3	1:61:A:LEU:HD21	7	0.13
(1,3004)	1:69:A:MET:HE3	1:61:A:LEU:HD22	7	0.13
(1,3004)	1:69:A:MET:HE3	1:61:A:LEU:HD23	7	0.13
(1,2930)	1:61:A:LEU:HD11	1:66:A:ILE:H	2	0.13
(1,2930)	1:61:A:LEU:HD12	1:66:A:ILE:H	2	0.13
(1,2930)	1:61:A:LEU:HD13	1:66:A:ILE:H	2	0.13
(1,2890)	1:129:A:LYS:HB2	1:130:A:GLY:H	6	0.13
(1,2857)	1:30:A:GLN:HE22	1:30:A:GLN:HB2	4	0.13
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	9	0.13
(1,2677)	1:14:A:ILE:HG13	1:16:A:ASN:H	9	0.13
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB1	8	0.13
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB2	8	0.13
(1,2625)	1:132:A:ILE:HB	1:125:A:ALA:HB3	8	0.13
(1,2467)	1:125:A:ALA:H	1:130:A:GLY:H	2	0.13
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	6	0.13
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	6	0.13
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	6	0.13
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	6	0.13
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	6	0.13
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	6	0.13
(1,2296)	1:37:A:PHE:HA	1:38:A:LEU:H	6	0.13
(1,2296)	1:37:A:PHE:HA	1:38:A:LEU:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2227)	1:132:A:ILE:HA	1:125:A:ALA:HB1	6	0.13
(1,2227)	1:132:A:ILE:HA	1:125:A:ALA:HB2	6	0.13
(1,2227)	1:132:A:ILE:HA	1:125:A:ALA:HB3	6	0.13
(1,2155)	1:125:A:ALA:HA	1:126:A:GLU:H	5	0.13
(1,2155)	1:125:A:ALA:HA	1:126:A:GLU:H	9	0.13
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	5	0.13
(1,2101)	1:140:A:GLU:HB3	1:169:A:GLN:HE22	7	0.13
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG11	1	0.13
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG12	1	0.13
(1,2057)	1:95:A:ARG:H	1:94:A:VAL:HG13	1	0.13
(1,2034)	1:10:A:GLU:HG2	1:10:A:GLU:H	9	0.13
(1,1890)	1:120:A:PHE:H	1:120:A:PHE:HD1	7	0.13
(1,1890)	1:120:A:PHE:H	1:120:A:PHE:HD2	7	0.13
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD11	6	0.13
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD12	6	0.13
(1,1869)	1:144:A:ASP:HB2	1:67:A:LEU:HD13	6	0.13
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	9	0.13
(1,1775)	1:162:A:ILE:HG21	1:182:A:GLU:H	4	0.13
(1,1775)	1:162:A:ILE:HG22	1:182:A:GLU:H	4	0.13
(1,1775)	1:162:A:ILE:HG23	1:182:A:GLU:H	4	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB1	1	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB2	1	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB3	1	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB1	10	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB2	10	0.13
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB3	10	0.13
(1,1693)	1:48:A:THR:HG1	1:48:A:THR:H	6	0.13
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG11	9	0.13
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG12	9	0.13
(1,1687)	1:160:A:THR:HG21	1:94:A:VAL:HG13	9	0.13
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG11	9	0.13
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG12	9	0.13
(1,1687)	1:160:A:THR:HG22	1:94:A:VAL:HG13	9	0.13
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG11	9	0.13
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG12	9	0.13
(1,1687)	1:160:A:THR:HG23	1:94:A:VAL:HG13	9	0.13
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	1	0.13
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	1	0.13
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	1	0.13
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	1	0.13
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	1	0.13
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	1	0.13
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	1	0.13
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	1	0.13
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG21	6	0.13
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG22	6	0.13
(1,1545)	1:156:A:GLN:HE22	1:152:A:THR:HG23	6	0.13
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD11	8	0.13
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD12	8	0.13
(1,1538)	1:41:A:ILE:HG13	1:38:A:LEU:HD13	8	0.13
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD2	1	0.13
(1,1507)	1:176:A:HIS:H	1:170:A:ARG:HD3	1	0.13
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	4	0.13
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	4	0.13
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	4	0.13
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG21	9	0.13
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG22	9	0.13
(1,1373)	1:50:A:ASP:H	1:48:A:THR:HG23	9	0.13
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD11	5	0.13
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD12	5	0.13
(1,1286)	1:150:A:ILE:HG21	1:147:A:ILE:HD13	5	0.13
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD11	5	0.13
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD12	5	0.13
(1,1286)	1:150:A:ILE:HG22	1:147:A:ILE:HD13	5	0.13
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD11	5	0.13
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD12	5	0.13
(1,1286)	1:150:A:ILE:HG23	1:147:A:ILE:HD13	5	0.13
(1,1274)	1:5:A:VAL:HG11	1:5:A:VAL:H	6	0.13
(1,1274)	1:5:A:VAL:HG12	1:5:A:VAL:H	6	0.13
(1,1274)	1:5:A:VAL:HG13	1:5:A:VAL:H	6	0.13
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	7	0.13
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	7	0.13
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	7	0.13
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	7	0.13
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	7	0.13
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	7	0.13
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	7	0.13
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	7	0.13
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	7	0.13
(1,1121)	1:84:A:ASP:H	1:82:A:GLY:H	4	0.13
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD11	3	0.13
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD12	3	0.13
(1,1097)	1:179:A:PHE:HD1	1:133:A:LEU:HD13	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD11	3	0.13
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD12	3	0.13
(1,1097)	1:179:A:PHE:HD2	1:133:A:LEU:HD13	3	0.13
(1,1053)	1:162:A:ILE:HA	1:164:A:MET:H	4	0.13
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	2	0.13
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	5	0.13
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD11	9	0.13
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD12	9	0.13
(1,919)	1:150:A:ILE:HA	1:150:A:ILE:HD13	9	0.13
(1,822)	1:179:A:PHE:HD1	1:133:A:LEU:HD21	4	0.13
(1,822)	1:179:A:PHE:HD1	1:133:A:LEU:HD22	4	0.13
(1,822)	1:179:A:PHE:HD1	1:133:A:LEU:HD23	4	0.13
(1,822)	1:179:A:PHE:HD2	1:133:A:LEU:HD21	4	0.13
(1,822)	1:179:A:PHE:HD2	1:133:A:LEU:HD22	4	0.13
(1,822)	1:179:A:PHE:HD2	1:133:A:LEU:HD23	4	0.13
(1,794)	1:136:A:TYR:HD1	1:177:A:THR:H	9	0.13
(1,794)	1:136:A:TYR:HD2	1:177:A:THR:H	9	0.13
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD21	10	0.13
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD22	10	0.13
(1,727)	1:150:A:ILE:HB	1:98:A:LEU:HD23	10	0.13
(1,566)	1:61:A:LEU:H	1:57:A:LYS:H	8	0.13
(1,528)	1:175:A:ASP:HB2	1:176:A:HIS:H	7	0.13
(1,528)	1:175:A:ASP:HB3	1:176:A:HIS:H	7	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	1	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	1	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	1	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	1	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	1	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	1	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	2	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	2	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	2	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	2	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	2	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	2	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	3	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	3	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	3	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	3	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	3	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	3	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	4	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	4	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	4	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	4	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	4	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	5	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	5	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	5	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	5	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	5	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	5	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	6	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	6	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	6	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	6	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	6	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	6	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	7	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	7	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	7	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	7	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	7	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	7	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	8	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	8	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	8	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	8	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	8	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	8	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	9	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	9	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	9	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	9	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	9	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	9	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD11	10	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD12	10	0.13
(1,422)	1:42:A:ILE:HG12	1:42:A:ILE:HD13	10	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD11	10	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD12	10	0.13
(1,422)	1:42:A:ILE:HG13	1:42:A:ILE:HD13	10	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	4	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	4	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	5	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	5	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	5	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	7	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	7	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	7	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	8	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	8	0.13
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	8	0.13
(1,328)	1:104:A:LEU:HD21	2:201:A:Z90:HAM	9	0.13
(1,328)	1:104:A:LEU:HD22	2:201:A:Z90:HAM	9	0.13
(1,328)	1:104:A:LEU:HD23	2:201:A:Z90:HAM	9	0.13
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG11	2	0.13
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG12	2	0.13
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG13	2	0.13
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG21	2	0.13
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG22	2	0.13
(1,324)	2:201:A:Z90:HAI	1:146:A:VAL:HG23	2	0.13
(1,313)	1:39:A:VAL:HG21	2:201:A:Z90:HAE	4	0.13
(1,313)	1:39:A:VAL:HG22	2:201:A:Z90:HAE	4	0.13
(1,313)	1:39:A:VAL:HG23	2:201:A:Z90:HAE	4	0.13
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG11	5	0.13
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG12	5	0.13
(1,306)	2:201:A:Z90:HAT	1:5:A:VAL:HG13	5	0.13
(1,299)	2:201:A:Z90:HAM	2:201:A:Z90:HBDA	7	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	1	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	1	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	2	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	2	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	3	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	3	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	6	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	6	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	8	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	8	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	10	0.13
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	10	0.13
(1,271)	1:150:A:ILE:HD11	2:201:A:Z90:HAI	3	0.13
(1,271)	1:150:A:ILE:HD12	2:201:A:Z90:HAI	3	0.13
(1,271)	1:150:A:ILE:HD13	2:201:A:Z90:HAI	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:101:A:LEU:HD21	2:201:A:Z90:HAI	10	0.13
(1,268)	1:101:A:LEU:HD22	2:201:A:Z90:HAI	10	0.13
(1,268)	1:101:A:LEU:HD23	2:201:A:Z90:HAI	10	0.13
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG11	4	0.13
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG12	4	0.13
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG13	4	0.13
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG21	4	0.13
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG22	4	0.13
(1,228)	1:64:A:GLY:H	1:52:A:VAL:HG23	4	0.13
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG12	2	0.13
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG13	2	0.13
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG12	3	0.13
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG13	3	0.13
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	10	0.13
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	10	0.13
(1,3573)	1:22:A:TRP:HE3	1:26:A:LYS:HB2	1	0.12
(1,3540)	1:54:A:ALA:HB1	1:28:A:GLU:H	6	0.12
(1,3540)	1:54:A:ALA:HB2	1:28:A:GLU:H	6	0.12
(1,3540)	1:54:A:ALA:HB3	1:28:A:GLU:H	6	0.12
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	2	0.12
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	2	0.12
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD21	2	0.12
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD22	2	0.12
(1,3403)	1:59:A:LEU:HD11	1:61:A:LEU:HD23	2	0.12
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD21	2	0.12
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD22	2	0.12
(1,3403)	1:59:A:LEU:HD12	1:61:A:LEU:HD23	2	0.12
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD21	2	0.12
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD22	2	0.12
(1,3403)	1:59:A:LEU:HD13	1:61:A:LEU:HD23	2	0.12
(1,3402)	1:49:A:TYR:HA	1:48:A:THR:H	10	0.12
(1,3358)	1:75:A:PHE:HE1	1:157:A:ILE:H	1	0.12
(1,3358)	1:75:A:PHE:HE2	1:157:A:ILE:H	1	0.12
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG21	3	0.12
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG22	3	0.12
(1,3338)	1:132:A:ILE:HA	1:132:A:ILE:HG23	3	0.12
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD11	9	0.12
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD12	9	0.12
(1,3312)	1:62:A:ASN:H	1:61:A:LEU:HD13	9	0.12
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD11	3	0.12
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD12	3	0.12
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD13	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3219)	1:162:A:ILE:HG13	1:154:A:ALA:H	3	0.12
(1,3183)	1:175:A:ASP:H	1:174:A:CYS:HB2	8	0.12
(1,3145)	1:58:A:VAL:HB	1:60:A:ASN:H	5	0.12
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	9	0.12
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	9	0.12
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	9	0.12
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	2	0.12
(1,3099)	1:8:A:ALA:HB1	1:12:A:LEU:H	8	0.12
(1,3099)	1:8:A:ALA:HB2	1:12:A:LEU:H	8	0.12
(1,3099)	1:8:A:ALA:HB3	1:12:A:LEU:H	8	0.12
(1,3003)	1:180:A:LEU:HB2	1:165:A:LYS:H	9	0.12
(1,3001)	1:137:A:SER:H	1:136:A:TYR:HB2	6	0.12
(1,2886)	1:134:A:HIS:HD2	1:134:A:HIS:H	3	0.12
(1,2698)	1:93:A:ASN:HA	1:94:A:VAL:H	3	0.12
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB1	1	0.12
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB2	1	0.12
(1,2674)	1:127:A:LYS:H	1:125:A:ALA:HB3	1	0.12
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	4	0.12
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	4	0.12
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	4	0.12
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	4	0.12
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	4	0.12
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	4	0.12
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB1	1	0.12
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB2	1	0.12
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB3	1	0.12
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB1	6	0.12
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB2	6	0.12
(1,2298)	1:150:A:ILE:HB	1:154:A:ALA:HB3	6	0.12
(1,2247)	1:174:A:CYS:H	1:174:A:CYS:HB3	2	0.12
(1,2247)	1:174:A:CYS:H	1:174:A:CYS:HB3	4	0.12
(1,1872)	1:136:A:TYR:HB2	1:135:A:TYR:H	4	0.12
(1,1848)	1:26:A:LYS:HB3	1:22:A:TRP:HE1	7	0.12
(1,1832)	1:19:A:PRO:HB3	1:20:A:GLU:H	6	0.12
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB1	5	0.12
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB2	5	0.12
(1,1831)	1:59:A:LEU:H	1:55:A:ALA:HB3	5	0.12
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	5	0.12
(1,1787)	1:176:A:HIS:HD2	1:179:A:PHE:H	9	0.12
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG21	5	0.12
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG22	5	0.12
(1,1588)	1:184:A:LYS:HA	1:162:A:ILE:HG23	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:164:A:MET:HE1	1:181:A:ILE:HB	8	0.12
(1,1582)	1:164:A:MET:HE2	1:181:A:ILE:HB	8	0.12
(1,1582)	1:164:A:MET:HE3	1:181:A:ILE:HB	8	0.12
(1,1582)	1:164:A:MET:HE1	1:181:A:ILE:HB	9	0.12
(1,1582)	1:164:A:MET:HE2	1:181:A:ILE:HB	9	0.12
(1,1582)	1:164:A:MET:HE3	1:181:A:ILE:HB	9	0.12
(1,1539)	1:1:A:MET:HE1	1:5:A:VAL:HB	9	0.12
(1,1539)	1:1:A:MET:HE2	1:5:A:VAL:HB	9	0.12
(1,1539)	1:1:A:MET:HE3	1:5:A:VAL:HB	9	0.12
(1,1503)	1:61:A:LEU:H	1:66:A:ILE:HD11	1	0.12
(1,1503)	1:61:A:LEU:H	1:66:A:ILE:HD12	1	0.12
(1,1503)	1:61:A:LEU:H	1:66:A:ILE:HD13	1	0.12
(1,1495)	1:125:A:ALA:HB1	1:131:A:LEU:H	10	0.12
(1,1495)	1:125:A:ALA:HB2	1:131:A:LEU:H	10	0.12
(1,1495)	1:125:A:ALA:HB3	1:131:A:LEU:H	10	0.12
(1,1437)	1:27:A:LYS:HB2	1:25:A:ILE:H	10	0.12
(1,1437)	1:27:A:LYS:HB3	1:25:A:ILE:H	10	0.12
(1,1404)	1:50:A:ASP:HB3	1:49:A:TYR:H	9	0.12
(1,1116)	1:160:A:THR:HB	1:155:A:GLN:HA	2	0.12
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD21	4	0.12
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD22	4	0.12
(1,1092)	1:12:A:LEU:H	1:9:A:LEU:HD23	4	0.12
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE1	4	0.12
(1,975)	1:44:A:ASP:H	1:43:A:TYR:HE2	4	0.12
(1,944)	1:162:A:ILE:HD11	1:164:A:MET:H	1	0.12
(1,944)	1:162:A:ILE:HD12	1:164:A:MET:H	1	0.12
(1,944)	1:162:A:ILE:HD13	1:164:A:MET:H	1	0.12
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	3	0.12
(1,904)	1:162:A:ILE:HB	1:151:A:LYS:HA	9	0.12
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD11	2	0.12
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD12	2	0.12
(1,813)	1:43:A:TYR:H	1:42:A:ILE:HD13	2	0.12
(1,767)	1:66:A:ILE:HG12	1:61:A:LEU:H	6	0.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD21	7	0.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD22	7	0.12
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD23	7	0.12
(1,703)	1:31:A:LEU:HB2	1:32:A:ASP:H	9	0.12
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG21	6	0.12
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG22	6	0.12
(1,702)	1:184:A:LYS:HB2	1:162:A:ILE:HG23	6	0.12
(1,460)	1:25:A:ILE:H	1:21:A:VAL:H	10	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	2	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	3	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	4	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	5	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	7	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	8	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	9	0.12
(1,250)	1:22:A:TRP:HE3	1:22:A:TRP:HH2	10	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG11	7	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG12	7	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG13	7	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG21	7	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG22	7	0.12
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG23	7	0.12
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG12	4	0.12
(1,204)	1:25:A:ILE:H	1:25:A:ILE:HG13	4	0.12
(1,179)	1:150:A:ILE:HG12	1:150:A:ILE:H	8	0.12
(1,179)	1:150:A:ILE:HG13	1:150:A:ILE:H	8	0.12
(1,3573)	1:22:A:TRP:HE3	1:26:A:LYS:HB2	6	0.11
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD11	10	0.11
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD12	10	0.11
(1,3487)	1:98:A:LEU:HA	1:98:A:LEU:HD13	10	0.11
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG2	8	0.11
(1,3480)	1:116:A:ARG:HE	1:116:A:ARG:HG3	8	0.11
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	5	0.11
(1,3402)	1:49:A:TYR:HA	1:48:A:THR:H	3	0.11
(1,3402)	1:49:A:TYR:HA	1:48:A:THR:H	7	0.11
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD11	7	0.11
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD12	7	0.11
(1,3373)	2:201:A:Z90:HAM	1:150:A:ILE:HD13	7	0.11
(1,3289)	1:63:A:ALA:HB1	1:67:A:LEU:H	8	0.11
(1,3289)	1:63:A:ALA:HB2	1:67:A:LEU:H	8	0.11
(1,3289)	1:63:A:ALA:HB3	1:67:A:LEU:H	8	0.11
(1,3257)	1:4:A:PHE:H	1:39:A:VAL:HG11	10	0.11
(1,3257)	1:4:A:PHE:H	1:39:A:VAL:HG12	10	0.11
(1,3257)	1:4:A:PHE:H	1:39:A:VAL:HG13	10	0.11
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD11	5	0.11
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD12	5	0.11
(1,3222)	1:60:A:ASN:H	1:59:A:LEU:HD13	5	0.11
(1,3181)	1:61:A:LEU:H	1:59:A:LEU:HD21	6	0.11
(1,3181)	1:61:A:LEU:H	1:59:A:LEU:HD22	6	0.11
(1,3181)	1:61:A:LEU:H	1:59:A:LEU:HD23	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG11	7	0.11
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG12	7	0.11
(1,3130)	1:21:A:VAL:H	1:21:A:VAL:HG13	7	0.11
(1,3115)	1:162:A:ILE:HA	1:163:A:ASP:H	10	0.11
(1,3111)	1:162:A:ILE:HB	1:181:A:ILE:HG21	7	0.11
(1,3111)	1:162:A:ILE:HB	1:181:A:ILE:HG22	7	0.11
(1,3111)	1:162:A:ILE:HB	1:181:A:ILE:HG23	7	0.11
(1,3099)	1:8:A:ALA:HB1	1:12:A:LEU:H	9	0.11
(1,3099)	1:8:A:ALA:HB2	1:12:A:LEU:H	9	0.11
(1,3099)	1:8:A:ALA:HB3	1:12:A:LEU:H	9	0.11
(1,3001)	1:137:A:SER:H	1:136:A:TYR:HB2	8	0.11
(1,2943)	1:43:A:TYR:HD1	1:38:A:LEU:H	8	0.11
(1,2943)	1:43:A:TYR:HD2	1:38:A:LEU:H	8	0.11
(1,2897)	1:60:A:ASN:H	1:59:A:LEU:HD21	2	0.11
(1,2897)	1:60:A:ASN:H	1:59:A:LEU:HD22	2	0.11
(1,2897)	1:60:A:ASN:H	1:59:A:LEU:HD23	2	0.11
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD11	8	0.11
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD12	8	0.11
(1,2891)	1:64:A:GLY:HA3	1:67:A:LEU:HD13	8	0.11
(1,2874)	1:77:A:PHE:H	1:73:A:MET:HE1	2	0.11
(1,2874)	1:77:A:PHE:H	1:73:A:MET:HE2	2	0.11
(1,2874)	1:77:A:PHE:H	1:73:A:MET:HE3	2	0.11
(1,2863)	1:126:A:GLU:H	1:130:A:GLY:H	5	0.11
(1,2798)	1:10:A:GLU:HA	1:22:A:TRP:HE1	5	0.11
(1,2781)	1:9:A:LEU:HD21	1:13:A:VAL:H	7	0.11
(1,2781)	1:9:A:LEU:HD22	1:13:A:VAL:H	7	0.11
(1,2781)	1:9:A:LEU:HD23	1:13:A:VAL:H	7	0.11
(1,2776)	1:26:A:LYS:H	1:22:A:TRP:HE1	2	0.11
(1,2759)	1:37:A:PHE:HD1	1:22:A:TRP:HE1	3	0.11
(1,2759)	1:37:A:PHE:HD2	1:22:A:TRP:HE1	3	0.11
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE1	6	0.11
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE2	6	0.11
(1,2721)	1:76:A:VAL:HG11	1:73:A:MET:HE3	6	0.11
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE1	6	0.11
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE2	6	0.11
(1,2721)	1:76:A:VAL:HG12	1:73:A:MET:HE3	6	0.11
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE1	6	0.11
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE2	6	0.11
(1,2721)	1:76:A:VAL:HG13	1:73:A:MET:HE3	6	0.11
(1,2712)	1:83:A:TYR:H	1:82:A:GLY:HA2	10	0.11
(1,2702)	1:52:A:VAL:HB	1:53:A:ALA:H	3	0.11
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB1	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB2	9	0.11
(1,2623)	1:124:A:ASP:HB2	1:125:A:ALA:HB3	9	0.11
(1,2492)	1:99:A:GLN:HB2	1:98:A:LEU:H	9	0.11
(1,2446)	1:108:A:LEU:HD11	1:108:A:LEU:HA	2	0.11
(1,2446)	1:108:A:LEU:HD12	1:108:A:LEU:HA	2	0.11
(1,2446)	1:108:A:LEU:HD13	1:108:A:LEU:HA	2	0.11
(1,2446)	1:108:A:LEU:HD21	1:108:A:LEU:HA	2	0.11
(1,2446)	1:108:A:LEU:HD22	1:108:A:LEU:HA	2	0.11
(1,2446)	1:108:A:LEU:HD23	1:108:A:LEU:HA	2	0.11
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD21	4	0.11
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD22	4	0.11
(1,2387)	1:6:A:ASN:H	1:9:A:LEU:HD23	4	0.11
(1,2169)	1:186:A:SER:H	1:184:A:LYS:HA	6	0.11
(1,2159)	1:131:A:LEU:HA	1:126:A:GLU:H	4	0.11
(1,2155)	1:125:A:ALA:HA	1:126:A:GLU:H	10	0.11
(1,2138)	1:174:A:CYS:H	1:171:A:ASN:HA	9	0.11
(1,2121)	1:174:A:CYS:HA	1:173:A:GLU:H	3	0.11
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG21	1	0.11
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG22	1	0.11
(1,2119)	1:165:A:LYS:HD3	1:167:A:ILE:HG23	1	0.11
(1,2065)	1:17:A:TYR:HB2	1:21:A:VAL:HG21	7	0.11
(1,2065)	1:17:A:TYR:HB2	1:21:A:VAL:HG22	7	0.11
(1,2065)	1:17:A:TYR:HB2	1:21:A:VAL:HG23	7	0.11
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG11	6	0.11
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG12	6	0.11
(1,2050)	1:158:A:HIS:H	1:153:A:VAL:HG13	6	0.11
(1,2029)	1:162:A:ILE:HG12	1:163:A:ASP:H	1	0.11
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB1	8	0.11
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB2	8	0.11
(1,1995)	1:160:A:THR:HB	1:154:A:ALA:HB3	8	0.11
(1,1947)	1:37:A:PHE:H	1:37:A:PHE:HD1	10	0.11
(1,1947)	1:37:A:PHE:H	1:37:A:PHE:HD2	10	0.11
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	7	0.11
(1,1817)	1:66:A:ILE:HB	1:56:A:SER:H	2	0.11
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB1	8	0.11
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB2	8	0.11
(1,1769)	1:181:A:ILE:H	1:125:A:ALA:HB3	8	0.11
(1,1738)	1:176:A:HIS:HD2	1:135:A:TYR:H	5	0.11
(1,1733)	1:49:A:TYR:HD1	1:142:A:LEU:H	3	0.11
(1,1733)	1:49:A:TYR:HD2	1:142:A:LEU:H	3	0.11
(1,1599)	1:176:A:HIS:H	1:174:A:CYS:H	1	0.11
(1,1587)	1:110:A:THR:HG21	1:110:A:THR:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1587)	1:110:A:THR:HG22	1:110:A:THR:H	6	0.11
(1,1587)	1:110:A:THR:HG23	1:110:A:THR:H	6	0.11
(1,1475)	1:56:A:SER:HB3	1:55:A:ALA:H	10	0.11
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD11	2	0.11
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD12	2	0.11
(1,1443)	1:159:A:GLY:H	1:157:A:ILE:HD13	2	0.11
(1,1409)	1:14:A:ILE:HB	1:18:A:GLY:H	3	0.11
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD11	6	0.11
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD12	6	0.11
(1,1230)	1:7:A:HIS:HD2	1:11:A:LEU:HD13	6	0.11
(1,1222)	1:152:A:THR:HA	1:154:A:ALA:HB1	6	0.11
(1,1222)	1:152:A:THR:HA	1:154:A:ALA:HB2	6	0.11
(1,1222)	1:152:A:THR:HA	1:154:A:ALA:HB3	6	0.11
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG21	1	0.11
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG22	1	0.11
(1,1215)	1:183:A:GLU:HA	1:162:A:ILE:HG23	1	0.11
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD21	10	0.11
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD22	10	0.11
(1,1209)	1:145:A:ILE:HG21	1:67:A:LEU:HD23	10	0.11
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD21	10	0.11
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD22	10	0.11
(1,1209)	1:145:A:ILE:HG22	1:67:A:LEU:HD23	10	0.11
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD21	10	0.11
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD22	10	0.11
(1,1209)	1:145:A:ILE:HG23	1:67:A:LEU:HD23	10	0.11
(1,1179)	1:167:A:ILE:HG12	1:179:A:PHE:H	3	0.11
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD11	5	0.11
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD12	5	0.11
(1,1157)	1:146:A:VAL:HB	1:133:A:LEU:HD13	5	0.11
(1,1071)	1:32:A:ASP:HA	1:31:A:LEU:HB3	2	0.11
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD11	4	0.11
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD12	4	0.11
(1,1064)	1:61:A:LEU:HB3	1:59:A:LEU:HD13	4	0.11
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE1	3	0.11
(1,960)	1:164:A:MET:HE1	1:179:A:PHE:HE2	3	0.11
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE1	3	0.11
(1,960)	1:164:A:MET:HE2	1:179:A:PHE:HE2	3	0.11
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE1	3	0.11
(1,960)	1:164:A:MET:HE3	1:179:A:PHE:HE2	3	0.11
(1,944)	1:162:A:ILE:HD11	1:164:A:MET:H	7	0.11
(1,944)	1:162:A:ILE:HD12	1:164:A:MET:H	7	0.11
(1,944)	1:162:A:ILE:HD13	1:164:A:MET:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:159:A:GLY:HA3	1:158:A:HIS:H	7	0.11
(1,753)	1:51:A:LEU:HD21	1:26:A:LYS:H	5	0.11
(1,753)	1:51:A:LEU:HD22	1:26:A:LYS:H	5	0.11
(1,753)	1:51:A:LEU:HD23	1:26:A:LYS:H	5	0.11
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD21	3	0.11
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD22	3	0.11
(1,740)	1:131:A:LEU:HB3	1:98:A:LEU:HD23	3	0.11
(1,730)	1:22:A:TRP:HH2	1:26:A:LYS:HB2	4	0.11
(1,718)	1:160:A:THR:HG21	1:159:A:GLY:H	3	0.11
(1,718)	1:160:A:THR:HG22	1:159:A:GLY:H	3	0.11
(1,718)	1:160:A:THR:HG23	1:159:A:GLY:H	3	0.11
(1,567)	1:173:A:GLU:H	1:171:A:ASN:H	8	0.11
(1,439)	1:118:A:PRO:HA	1:119:A:SER:H	5	0.11
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG11	9	0.11
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG12	9	0.11
(1,418)	1:155:A:GLN:H	1:94:A:VAL:HG13	9	0.11
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD21	3	0.11
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD22	3	0.11
(1,392)	1:31:A:LEU:HB3	1:31:A:LEU:HD23	3	0.11
(1,311)	1:39:A:VAL:HG11	2:201:A:Z90:HAE	7	0.11
(1,311)	1:39:A:VAL:HG12	2:201:A:Z90:HAE	7	0.11
(1,311)	1:39:A:VAL:HG13	2:201:A:Z90:HAE	7	0.11
(1,307)	1:5:A:VAL:HG11	2:201:A:Z90:HAR	10	0.11
(1,307)	1:5:A:VAL:HG12	2:201:A:Z90:HAR	10	0.11
(1,307)	1:5:A:VAL:HG13	2:201:A:Z90:HAR	10	0.11
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	5	0.11
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	5	0.11
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAY	9	0.11
(1,291)	2:201:A:Z90:HAJ	2:201:A:Z90:HAYA	9	0.11
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG21	1	0.11
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG22	1	0.11
(1,276)	2:201:A:Z90:HAF	1:39:A:VAL:HG23	1	0.11
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD21	3	0.11
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD22	3	0.11
(1,252)	1:22:A:TRP:HE3	1:51:A:LEU:HD23	3	0.11
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG11	4	0.11
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG12	4	0.11
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG13	4	0.11
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG21	4	0.11
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG22	4	0.11
(1,248)	1:54:A:ALA:H	1:52:A:VAL:HG23	4	0.11
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG12	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:59:A:LEU:H	1:25:A:ILE:HG13	10	0.11
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB1	8	0.11
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB2	8	0.11
(1,219)	1:56:A:SER:H	1:54:A:ALA:HB3	8	0.11
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD11	10	0.11
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD12	10	0.11
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD13	10	0.11
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD21	10	0.11
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD22	10	0.11
(1,216)	1:33:A:GLU:H	1:31:A:LEU:HD23	10	0.11
(1,161)	1:171:A:ASN:HD22	1:171:A:ASN:H	9	0.11
(1,137)	1:65:A:GLU:HA	1:62:A:ASN:H	8	0.11
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB2	8	0.11
(1,14)	1:58:A:VAL:HB	1:57:A:LYS:HB3	8	0.11
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD21	2	0.1
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD22	2	0.1
(1,3469)	1:55:A:ALA:HB1	1:9:A:LEU:HD23	2	0.1
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD21	2	0.1
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD22	2	0.1
(1,3469)	1:55:A:ALA:HB2	1:9:A:LEU:HD23	2	0.1
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD21	2	0.1
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD22	2	0.1
(1,3469)	1:55:A:ALA:HB3	1:9:A:LEU:HD23	2	0.1
(1,3453)	1:30:A:GLN:HA	1:28:A:GLU:H	2	0.1
(1,3139)	1:160:A:THR:HB	1:94:A:VAL:HG21	1	0.1
(1,3139)	1:160:A:THR:HB	1:94:A:VAL:HG22	1	0.1
(1,3139)	1:160:A:THR:HB	1:94:A:VAL:HG23	1	0.1
(1,3099)	1:8:A:ALA:HB1	1:12:A:LEU:H	6	0.1
(1,3099)	1:8:A:ALA:HB2	1:12:A:LEU:H	6	0.1
(1,3099)	1:8:A:ALA:HB3	1:12:A:LEU:H	6	0.1
(1,3012)	1:176:A:HIS:H	1:174:A:CYS:HB3	7	0.1
(1,2703)	1:154:A:ALA:HB1	1:153:A:VAL:HG21	5	0.1
(1,2703)	1:154:A:ALA:HB1	1:153:A:VAL:HG22	5	0.1
(1,2703)	1:154:A:ALA:HB1	1:153:A:VAL:HG23	5	0.1
(1,2703)	1:154:A:ALA:HB2	1:153:A:VAL:HG21	5	0.1
(1,2703)	1:154:A:ALA:HB2	1:153:A:VAL:HG22	5	0.1
(1,2703)	1:154:A:ALA:HB2	1:153:A:VAL:HG23	5	0.1
(1,2703)	1:154:A:ALA:HB3	1:153:A:VAL:HG21	5	0.1
(1,2703)	1:154:A:ALA:HB3	1:153:A:VAL:HG22	5	0.1
(1,2703)	1:154:A:ALA:HB3	1:153:A:VAL:HG23	5	0.1
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB1	10	0.1
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2540)	1:52:A:VAL:HB	1:53:A:ALA:HB3	10	0.1
(1,2423)	1:183:A:GLU:HB3	1:184:A:LYS:H	1	0.1
(1,2328)	1:179:A:PHE:HA	1:179:A:PHE:HD1	8	0.1
(1,2328)	1:179:A:PHE:HA	1:179:A:PHE:HD2	8	0.1
(1,2130)	1:167:A:ILE:HG12	1:179:A:PHE:H	9	0.1
(1,2018)	1:44:A:ASP:HB3	1:47:A:LYS:H	5	0.1
(1,1894)	1:62:A:ASN:HD22	1:65:A:GLU:H	10	0.1
(1,1826)	1:21:A:VAL:HB	1:20:A:GLU:H	10	0.1
(1,1801)	1:94:A:VAL:HB	1:94:A:VAL:HA	10	0.1
(1,1621)	1:27:A:LYS:HG2	1:27:A:LYS:H	1	0.1
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD11	5	0.1
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD12	5	0.1
(1,1580)	1:41:A:ILE:HG21	1:38:A:LEU:HD13	5	0.1
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD11	5	0.1
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD12	5	0.1
(1,1580)	1:41:A:ILE:HG22	1:38:A:LEU:HD13	5	0.1
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD11	5	0.1
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD12	5	0.1
(1,1580)	1:41:A:ILE:HG23	1:38:A:LEU:HD13	5	0.1
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD11	9	0.1
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD12	9	0.1
(1,1174)	1:41:A:ILE:H	1:38:A:LEU:HD13	9	0.1
(1,1163)	1:153:A:VAL:HG11	1:153:A:VAL:H	9	0.1
(1,1163)	1:153:A:VAL:HG12	1:153:A:VAL:H	9	0.1
(1,1163)	1:153:A:VAL:HG13	1:153:A:VAL:H	9	0.1
(1,1141)	1:161:A:GLU:H	1:160:A:THR:HG21	5	0.1
(1,1141)	1:161:A:GLU:H	1:160:A:THR:HG22	5	0.1
(1,1141)	1:161:A:GLU:H	1:160:A:THR:HG23	5	0.1
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD11	10	0.1
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD12	10	0.1
(1,1112)	1:52:A:VAL:H	1:51:A:LEU:HD13	10	0.1
(1,1066)	1:139:A:ARG:HG3	1:140:A:GLU:H	2	0.1
(1,1035)	1:170:A:ARG:HE	1:170:A:ARG:HG3	5	0.1
(1,938)	1:122:A:CYS:HA	1:123:A:THR:H	1	0.1
(1,767)	1:66:A:ILE:HG12	1:61:A:LEU:H	3	0.1
(1,725)	1:94:A:VAL:H	1:94:A:VAL:HG21	7	0.1
(1,725)	1:94:A:VAL:H	1:94:A:VAL:HG22	7	0.1
(1,725)	1:94:A:VAL:H	1:94:A:VAL:HG23	7	0.1
(1,627)	1:92:A:SER:HB2	1:93:A:ASN:H	4	0.1

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

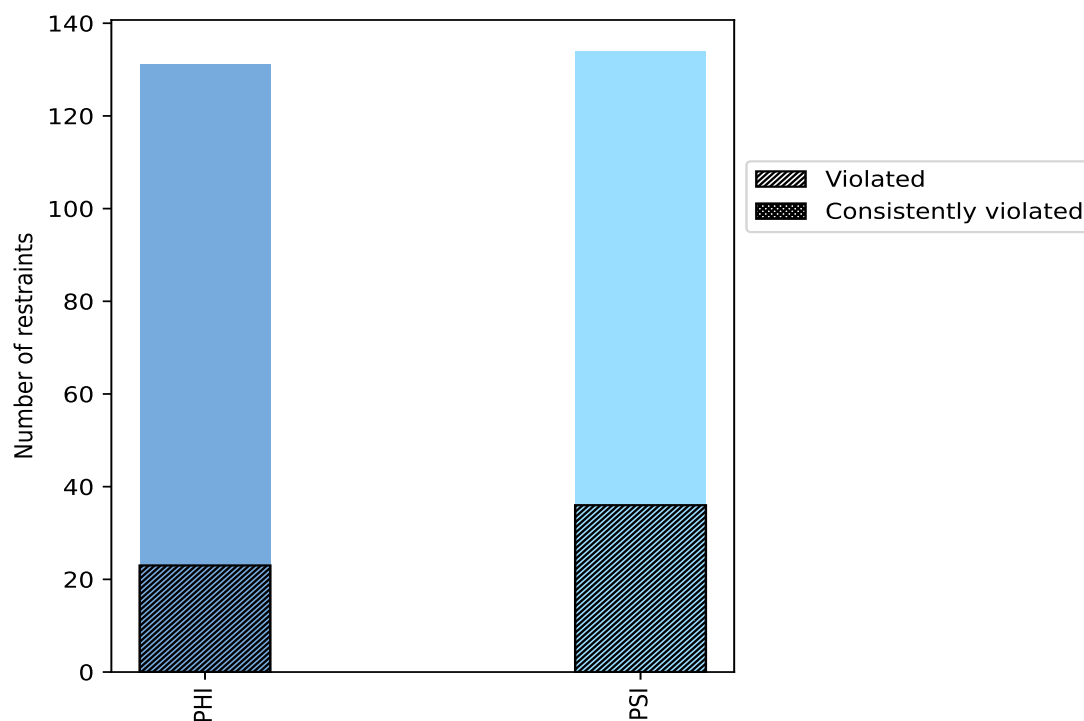
### 10.1 Summary of dihedral-angle violations [i](#)

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	131	49.4	23	17.6	8.7	0	0.0	0.0
PSI	134	50.6	36	26.9	13.6	0	0.0	0.0
Total	265	100.0	59	22.3	22.3	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](#)



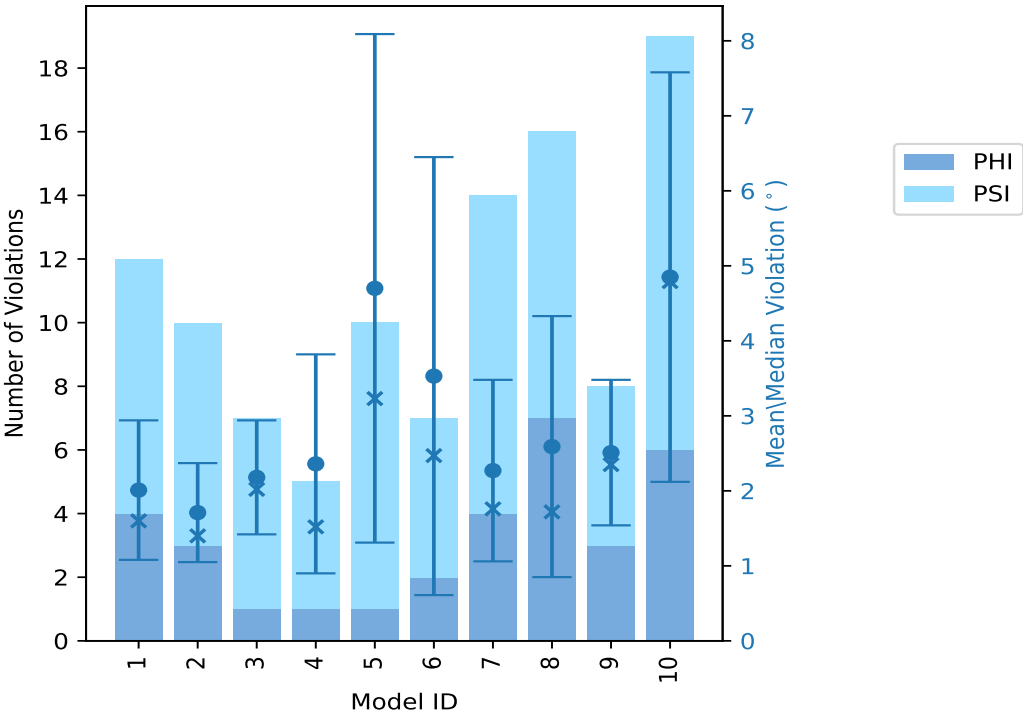
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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	4	8	12	2.01	3.62	0.93	1.6
2	3	7	10	1.71	3.23	0.66	1.4
3	1	6	7	2.18	3.64	0.76	2.02
4	1	4	5	2.36	4.73	1.46	1.52
5	1	9	10	4.7	11.19	3.39	3.23
6	2	5	7	3.53	10.16	2.92	2.47
7	4	10	14	2.27	5.66	1.21	1.76
8	7	9	16	2.59	6.1	1.74	1.72
9	3	5	8	2.51	4.08	0.97	2.35
10	6	13	19	4.85	9.32	2.73	4.79

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

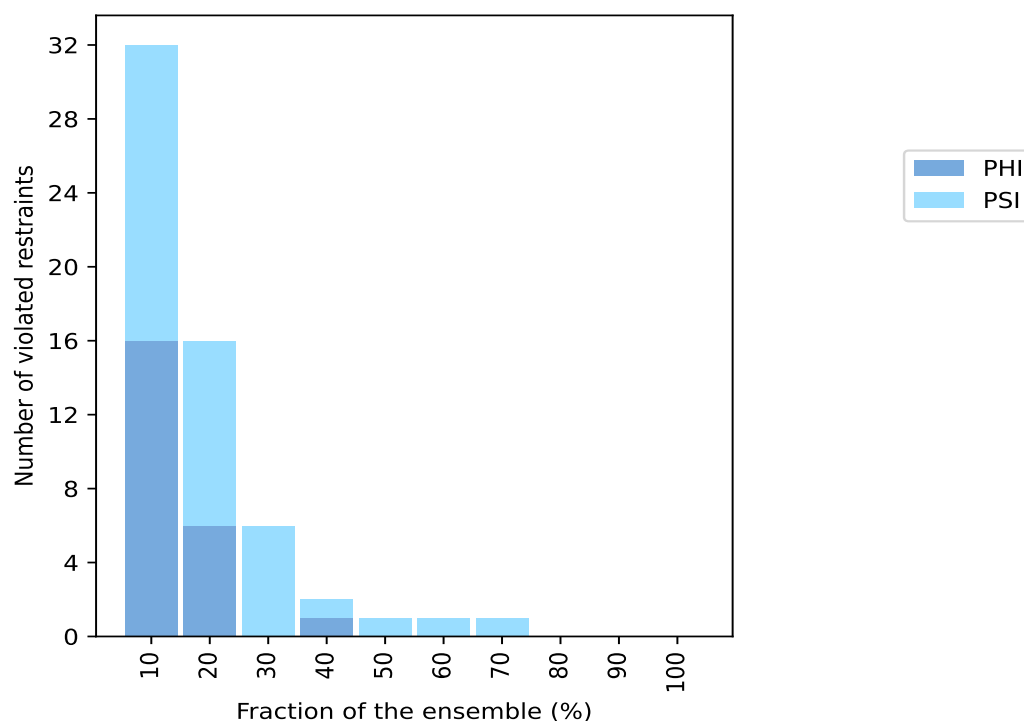
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
16	16	32	1	10.0
6	10	16	2	20.0
0	6	6	3	30.0
1	1	2	4	40.0
0	1	1	5	50.0
0	1	1	6	60.0
0	1	1	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

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

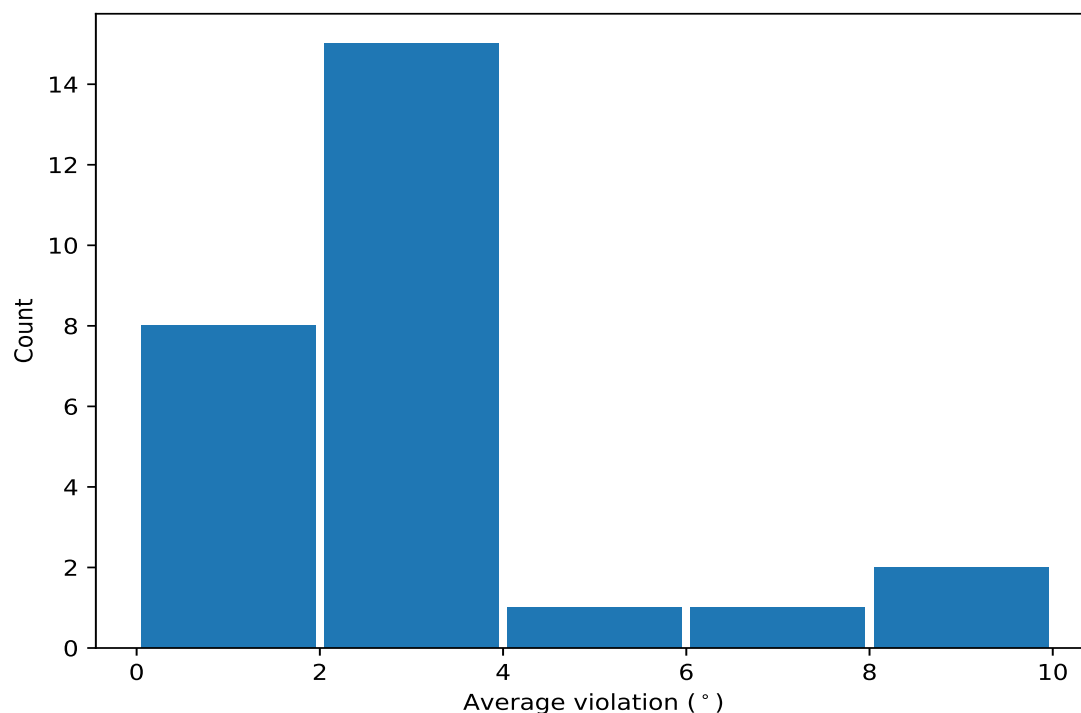
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	7	2.55	0.96	2.73
(1,121)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:ASP:N	6	2.76	0.91	2.88
(1,133)	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1:90:A:LEU:N	5	3.6	1.62	4.1
(1,181)	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	1:117:A:ALA:N	4	2.43	0.98	2.2
(1,130)	1:87:A:LEU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	4	1.71	0.17	1.74
(1,202)	1:134:A:HIS:N	1:134:A:HIS:CA	1:134:A:HIS:C	1:135:A:TYR:N	3	1.76	0.43	1.53
(1,175)	1:112:A:TYR:N	1:112:A:TYR:CA	1:112:A:TYR:C	1:113:A:PRO:N	3	1.57	0.64	1.17
(1,243)	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	1:164:A:MET:N	3	1.51	0.46	1.25
(1,263)	1:182:A:GLU:N	1:182:A:GLU:CA	1:182:A:GLU:C	1:183:A:GLU:N	3	1.47	0.25	1.37
(1,189)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:ARG:N	3	1.4	0.27	1.36
(1,131)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:VAL:N	3	1.23	0.12	1.23
(1,118)	1:81:A:SER:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	2	9.14	2.04	9.14
(1,117)	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	1:82:A:GLY:N	2	8.22	2.43	8.22

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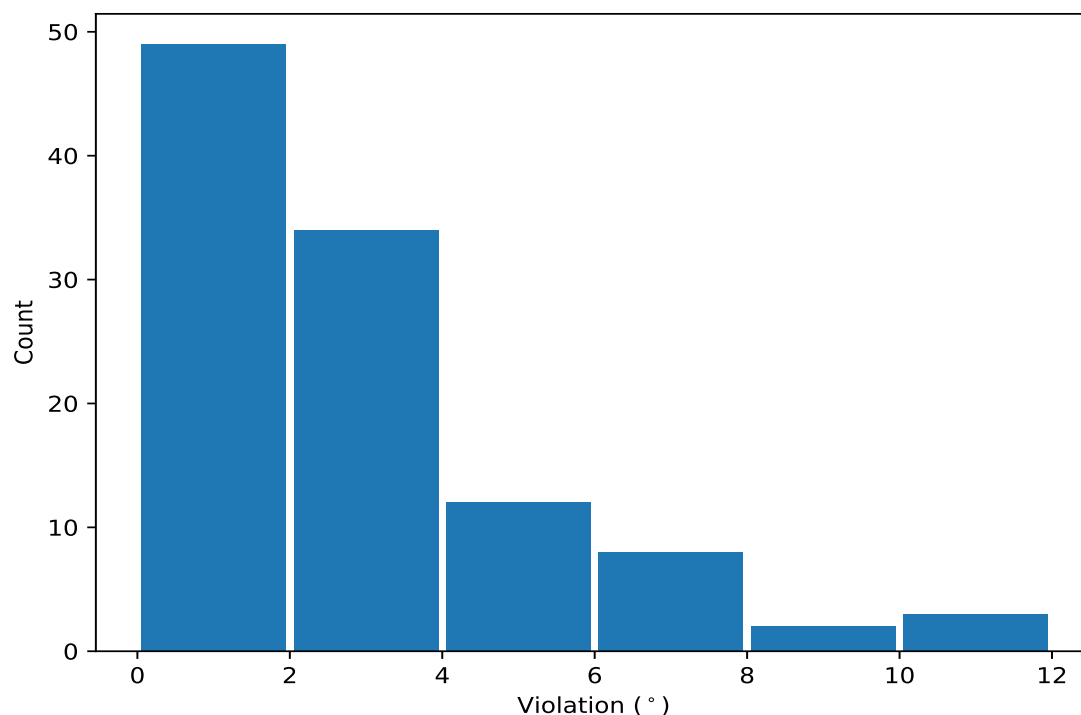
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,206)	1:136:A:TYR:N	1:136:A:TYR:CA	1:136:A:TYR:C	1:137:A:SER:N	2	6.63	3.53	6.63
(1,119)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:TYR:N	2	5.28	1.15	5.28
(1,115)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:SER:N	2	3.64	1.92	3.64
(1,129)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:ARG:N	2	3.02	1.76	3.02
(1,207)	1:136:A:TYR:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	2	2.82	1.7	2.82
(1,183)	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	1:118:A:PRO:N	2	2.68	0.68	2.68
(1,180)	1:115:A:MET:C	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	2	2.64	0.9	2.64
(1,185)	1:118:A:PRO:N	1:118:A:PRO:CA	1:118:A:PRO:C	1:119:A:SER:N	2	2.58	1.5	2.58
(1,135)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLY:N	2	2.26	0.96	2.26
(1,203)	1:134:A:HIS:C	1:135:A:TYR:N	1:135:A:TYR:CA	1:135:A:TYR:C	2	2.14	1.02	2.14
(1,125)	1:85:A:THR:N	1:85:A:THR:CA	1:85:A:THR:C	1:86:A:ILE:N	2	2.04	0.35	2.04
(1,196)	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	1:132:A:ILE:N	2	2.02	0.23	2.02
(1,182)	1:116:A:ARG:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	2	2.0	0.02	2.0
(1,134)	1:89:A:VAL:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	2	1.82	0.3	1.82

<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 (°)
(1,118)	1:81:A:SER:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	5	11.19
(1,117)	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	1:82:A:GLY:N	5	10.65
(1,206)	1:136:A:TYR:N	1:136:A:TYR:CA	1:136:A:TYR:C	1:137:A:SER:N	6	10.16
(1,172)	1:110:A:THR:C	1:111:A:ILE:N	1:111:A:ILE:CA	1:111:A:ILE:C	10	9.32
(1,169)	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	1:110:A:THR:N	10	8.61
(1,171)	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	1:111:A:ILE:N	10	7.86
(1,168)	1:108:A:LEU:C	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	10	7.76
(1,170)	1:109:A:ALA:C	1:110:A:THR:N	1:110:A:THR:CA	1:110:A:THR:C	10	7.52
(1,118)	1:81:A:SER:C	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	10	7.1
(1,173)	1:111:A:ILE:N	1:111:A:ILE:CA	1:111:A:ILE:C	1:112:A:TYR:N	10	6.58
(1,167)	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	1:109:A:ALA:N	10	6.52
(1,119)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:TYR:N	5	6.43
(1,116)	1:80:A:GLU:C	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	8	6.1
(1,117)	1:81:A:SER:N	1:81:A:SER:CA	1:81:A:SER:C	1:82:A:GLY:N	10	5.8
(1,133)	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1:90:A:LEU:N	7	5.66
(1,115)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:SER:N	8	5.57
(1,108)	1:76:A:VAL:C	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	8	5.55
(1,129)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:ARG:N	10	4.79
(1,133)	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1:90:A:LEU:N	4	4.73
(1,207)	1:136:A:TYR:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	6	4.52
(1,111)	1:78:A:CYS:N	1:78:A:CYS:CA	1:78:A:CYS:C	1:79:A:GLN:N	8	4.46
(1,119)	1:82:A:GLY:N	1:82:A:GLY:CA	1:82:A:GLY:C	1:83:A:TYR:N	10	4.13
(1,133)	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1:90:A:LEU:N	5	4.1
(1,185)	1:118:A:PRO:N	1:118:A:PRO:CA	1:118:A:PRO:C	1:119:A:SER:N	9	4.08
(1,181)	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	1:117:A:ALA:N	9	4.0
(1,121)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:ASP:N	5	3.73
(1,121)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:ASP:N	10	3.69
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	3	3.64
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	1	3.62
(1,1)	1:3:A:GLY:N	1:3:A:GLY:CA	1:3:A:GLY:C	1:4:A:PHE:N	7	3.56
(1,180)	1:115:A:MET:C	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	1	3.54
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	4	3.38
(1,183)	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	1:118:A:PRO:N	6	3.36
(1,112)	1:78:A:CYS:C	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	8	3.26
(1,135)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLY:N	2	3.23
(1,203)	1:134:A:HIS:C	1:135:A:TYR:N	1:135:A:TYR:CA	1:135:A:TYR:C	7	3.17
(1,206)	1:136:A:TYR:N	1:136:A:TYR:CA	1:136:A:TYR:C	1:137:A:SER:N	1	3.1
(1,121)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:ASP:N	7	2.98
(1,166)	1:107:A:HIS:C	1:108:A:LEU:N	1:108:A:LEU:CA	1:108:A:LEU:C	10	2.96
(1,121)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:ASP:N	3	2.78
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	5	2.73
(1,197)	1:131:A:LEU:C	1:132:A:ILE:N	1:132:A:ILE:CA	1:132:A:ILE:C	1	2.68
(1,124)	1:84:A:ASP:C	1:85:A:THR:N	1:85:A:THR:CA	1:85:A:THR:C	7	2.64
(1,175)	1:112:A:TYR:N	1:112:A:TYR:CA	1:112:A:TYR:C	1:113:A:PRO:N	6	2.47
(1,174)	1:111:A:ILE:C	1:112:A:TYR:N	1:112:A:TYR:CA	1:112:A:TYR:C	10	2.44
(1,125)	1:85:A:THR:N	1:85:A:THR:CA	1:85:A:THR:C	1:86:A:ILE:N	5	2.39
(1,202)	1:134:A:HIS:N	1:134:A:HIS:CA	1:134:A:HIS:C	1:135:A:TYR:N	9	2.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,121)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:ASP:N	9	2.36
(1,186)	1:118:A:PRO:C	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	9	2.34
(1,133)	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1:90:A:LEU:N	2	2.29
(1,181)	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	1:117:A:ALA:N	3	2.26
(1,196)	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	1:132:A:ILE:N	5	2.24
(1,114)	1:79:A:GLN:C	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	8	2.21
(1,243)	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	1:164:A:MET:N	5	2.16
(1,181)	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	1:117:A:ALA:N	2	2.15
(1,134)	1:89:A:VAL:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	7	2.12
(1,182)	1:116:A:ARG:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	2	2.02
(1,127)	1:86:A:ILE:N	1:86:A:ILE:CA	1:86:A:ILE:C	1:87:A:LEU:N	3	2.02
(1,183)	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	1:118:A:PRO:N	1	2.01
(1,182)	1:116:A:ARG:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	9	1.98
(1,130)	1:87:A:LEU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	9	1.9
(1,263)	1:182:A:GLU:N	1:182:A:GLU:CA	1:182:A:GLU:C	1:183:A:GLU:N	3	1.82
(1,130)	1:87:A:LEU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1	1.81
(1,196)	1:131:A:LEU:N	1:131:A:LEU:CA	1:131:A:LEU:C	1:132:A:ILE:N	6	1.79
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	8	1.78
(1,137)	1:91:A:GLY:N	1:91:A:GLY:CA	1:91:A:GLY:C	1:92:A:SER:N	7	1.77
(1,189)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:ARG:N	7	1.75
(1,180)	1:115:A:MET:C	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	8	1.75
(1,115)	1:80:A:GLU:N	1:80:A:GLU:CA	1:80:A:GLU:C	1:81:A:SER:N	10	1.72
(1,125)	1:85:A:THR:N	1:85:A:THR:CA	1:85:A:THR:C	1:86:A:ILE:N	8	1.7
(1,113)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:GLU:N	8	1.68
(1,130)	1:87:A:LEU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	8	1.66
(1,187)	1:119:A:SER:N	1:119:A:SER:CA	1:119:A:SER:C	1:120:A:PHE:N	7	1.56
(1,209)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:GLN:N	10	1.53
(1,202)	1:134:A:HIS:N	1:134:A:HIS:CA	1:134:A:HIS:C	1:135:A:TYR:N	7	1.53
(1,134)	1:89:A:VAL:C	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	4	1.52
(1,53)	1:45:A:ASP:N	1:45:A:ASP:CA	1:45:A:ASP:C	1:46:A:SER:N	7	1.48
(1,130)	1:87:A:LEU:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	3	1.46
(1,234)	1:154:A:ALA:C	1:155:A:GLN:N	1:155:A:GLN:CA	1:155:A:GLN:C	6	1.42
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	2	1.42
(1,202)	1:134:A:HIS:N	1:134:A:HIS:CA	1:134:A:HIS:C	1:135:A:TYR:N	1	1.4
(1,263)	1:182:A:GLU:N	1:182:A:GLU:CA	1:182:A:GLU:C	1:183:A:GLU:N	2	1.37
(1,131)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:VAL:N	5	1.37
(1,189)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:ARG:N	2	1.36
(1,181)	1:116:A:ARG:N	1:116:A:ARG:CA	1:116:A:ARG:C	1:117:A:ALA:N	10	1.32
(1,153)	1:100:A:ASN:N	1:100:A:ASN:CA	1:100:A:ASN:C	1:101:A:LEU:N	7	1.31
(1,135)	1:90:A:LEU:N	1:90:A:LEU:CA	1:90:A:LEU:C	1:91:A:GLY:N	1	1.3
(1,109)	1:77:A:PHE:N	1:77:A:PHE:CA	1:77:A:PHE:C	1:78:A:CYS:N	8	1.28
(1,129)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:ARG:N	7	1.26
(1,243)	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	1:164:A:MET:N	3	1.25
(1,263)	1:182:A:GLU:N	1:182:A:GLU:CA	1:182:A:GLU:C	1:183:A:GLU:N	10	1.23
(1,184)	1:117:A:ALA:C	1:118:A:PRO:N	1:118:A:PRO:CA	1:118:A:PRO:C	1	1.23
(1,131)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:VAL:N	10	1.23
(1,133)	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1:90:A:LEU:N	1	1.22
(1,175)	1:112:A:TYR:N	1:112:A:TYR:CA	1:112:A:TYR:C	1:113:A:PRO:N	1	1.17
(1,211)	1:143:A:GLN:N	1:143:A:GLN:CA	1:143:A:GLN:C	1:144:A:ASP:N	8	1.15
(1,141)	1:94:A:VAL:N	1:94:A:VAL:CA	1:94:A:VAL:C	1:95:A:ARG:N	2	1.15
(1,243)	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	1:164:A:MET:N	4	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,203)	1:134:A:HIS:C	1:135:A:TYR:N	1:135:A:TYR:CA	1:135:A:TYR:C	2	1.12
(1,207)	1:136:A:TYR:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	8	1.11
(1,185)	1:118:A:PRO:N	1:118:A:PRO:CA	1:118:A:PRO:C	1:119:A:SER:N	1	1.09
(1,189)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:ARG:N	8	1.08
(1,175)	1:112:A:TYR:N	1:112:A:TYR:CA	1:112:A:TYR:C	1:113:A:PRO:N	9	1.08
(1,131)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:VAL:N	8	1.08
(1,121)	1:83:A:TYR:N	1:83:A:TYR:CA	1:83:A:TYR:C	1:84:A:ASP:N	4	1.04
(1,262)	1:181:A:ILE:C	1:182:A:GLU:N	1:182:A:GLU:CA	1:182:A:GLU:C	2	1.02
(1,239)	1:161:A:GLU:N	1:161:A:GLU:CA	1:161:A:GLU:C	1:162:A:ILE:N	6	1.02
(1,242)	1:162:A:ILE:C	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	7	1.0